APPLYING THE PRINCIPLE OF CORRESPONDING STATES TO MULTI-COMPONENT HYDROCARBON MIXTURES (JET FUELS)

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APPLYING THE PRINCIPLE OF CORRESPONDING STATES TO MULTI-COMPONENT HYDROCARBON MIXTURES (JET FUELS)

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ABSTRACT

APPLYING THE PRINCIPLE OF CORRESPONDING STATES TO MULTI-COMPONENT HYDROCARBON MIXTURES (JET FUELS)

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Aviation turbine fuel is required to meet stringent product specifications due the critical importance it plays inside of the turbines during the fuel's use. The specification tests for military and commercial grades of jet fuel include over twenty individual analyses, which are costly in both time and money. In addition, these specifications were designed for petroleum derived fuels and are not always applicable to new finished fuels from alternative sources. For these reasons, it is desirable to develop tools to assess a broad range of jet fuel properties based on the underlying chemical composition. This work outlines a methodology to predict two fuel properties, i.e., density and viscosity, using a theoretical model called generalized corresponding states (GCSP), a subset of the corresponding states principal (CSP). The work analyzes different methods to calculate the critical properties of the mixtures' components. The components are of vital importance to GCSP. It also investigates reference fluids of the system, which is another important factor in modelling with GCSP. Results for the separate physical parameters, using an initial set of over 50 jet fuels, indicates model predictions fall within an average

error range that spans from 0.01% to 7.29%, and is strongly dependent on the critical properties and reference fluids used. Additional improvements to current models and methods are proposed.

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LIST OF SYMBOLS AND ABBREVIATIONS

Abbreviations

CSP – Corresponding States Principal

GCSP – Generalized CSP

GCxGC – Two-Dimensional Gas Chromatography

HPLC – High Performance Liquid Chromatography

DIPPR – Design Institute for Physical Properties

AIChE – American Institute of Chemical Engineers

EOS – Equation of State

AAD% - Absolute Average Deviation

Ave% - Average Error

Zone Err% - Error for a nominal temperature

Symbols

T – Temperature

P – Pressure

V – Volume

Z – Compressibility factor

ω – Acentric factor

X – Variable used in GCSP equations to represent property of interest

ρ – Density

η – Dynamic viscosity

θ – Variable used in Riazi/Daubert property estimation method to stand for the property of interest

MW – Molecular weight

α_{ij} – Binary interaction coefficient

CN – Carbon Number

GC – Gas chromatography response

x_i – Mole fraction

ξ – Viscosity reducing factor

v – Reduced volume

y_i – Point error

Δ – Error Statistic

Sub/Super Scripts

b – Boiling point

m – Mixture property

r – Reduced property

c – Critical point property

br – Reduced boiling point

cm – Mixture pseudo-critical property

(r#) – Reference fluid number

CHAPTER 1

INTRODUCTION

There are many types of useful mixtures in existence, but among the most widely used are hydrocarbon mixtures, e.g., oil and gas. These hydrocarbon mixtures are an important energy source for the transportation industry. The aviation sector alone consumed 5417.7 thousand barrels per day of fuel globally in 2012 (U.S. Energy Information Administration, 2015). Hydrocarbon fuels must typically meet some minimum amount of inherent energy requirements (typically measured as heat of combustion, ΔH_{comb}), but often must also meet other property specifications, e.g., density, viscosity, freeze point, and distillation, in order to satisfy the engineering requirements of a specific engine or platform using the fuel. Aviation turbine fuels, a subset of all hydrocarbon fuels, are highly specified and must satisfy an extensive list of chemical and physical properties to meet performance requirements associated with the high-stress environments of aviation. To meet these requirements a specific "cut" (industry term for distillation and refining process from crude oil) undergoes a battery of standardized tests to assure fuel quality. The experimental techniques used to evaluate fuels – often in the form of ASTM standard tests – can be costly in both time and money and can be limited in scope, e.g., only valid

for petroleum fuels (not alternative fuels) or measurements occur at just a single temperature. As such it is desirable to develop for use a single test that would be able to reduce and combine a large majority of the tests.

CHAPTER 2

BACKGROUND

2.1 Fuels Characterization

Jet fuel is a complex hydrocarbon mixture that contains hundreds of distinct compounds. Rather than identify every compound, or the specific chemical composition of every single batch of fuel, the jet fuel industry performs a series of specification tests to assure the quality of the fuel batch. For instance, ASTM D4052 is an experimental technique to measure the density of a fuel at a single, predetermined temperature (20 °C). If the density is within 0.775 to 0.840 g/mL, the fuel passes the density specification for Jet A fuel (ASTM D1655). Similar experimental checks are carried out for viscosity (ASTM D455), freeze point (ASTM D5972), flash point (ASTM D93), and so on. However, throughout these specification tests, property information is not collected over a comprehensive range of temperatures, i.e., the temperature dependence of a property is not determined. And additional fit-for-purpose (FFP) properties, i.e., properties that are required for aircraft operation, such as thermal conductivity, bulk modulus, and surface tension are not tested at all. These additional FFP properties are assumed to be satisfied

when the specifications are met. While this might be true for traditional petroleum-derived fuels, it may not necessarily be the case for alternative fuel formulations. To that end, investigating methods of determining all of these properties (specification and FFP) without each batch of fuel undergoing extensive tests is a worthwhile investment of resources.

2.1.1 Detailed Hydrocarbon Type via GCxGC

Chemical composition is often obtained from a separation method. One such method is GCxGC, which is a gas chromatography method that separates a mixture based on both volatility and polarity. Figure 1 shows a GCxGC chromatograph of a typical Jet A fuel. Both the x-axis and y-axis give a retention time; however, separation in the x-axis is based on volatility differences and separation in the y-axis is based on polarity differences. Color intensity indicates the amount of substance, where red is the highest relative intensity, followed by yellow, green, and blue (off-white is baseline). Compound and compound classes are identified by retention time locations and are quantified using flame ionization detection (FID). GCxGC is still a relatively new technique developed as an alternative to ASTM D2425, a technique that requires HPLC (high-performance liquid chromatography), and ASTM D2549. However, GCxGC has been demonstrated to provide high-fidelity composition information using very small volumes of fuel (< 1mL), with a relatively fast analysis time of about two to three hours (Striebich et al., 2014).

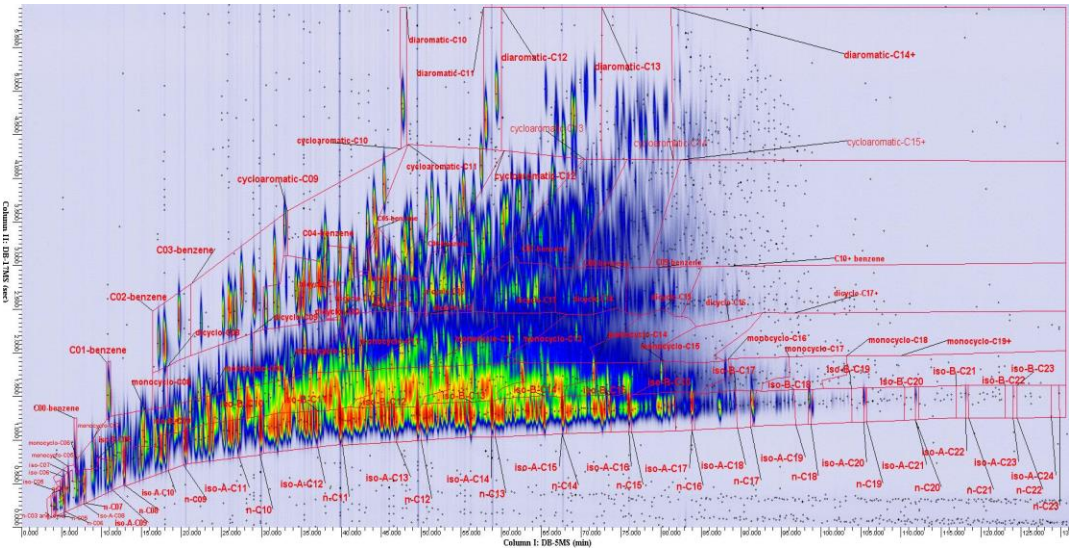

Figure 1. Sample GCxGC chromatograph of a Jet A fuel.

2.2 Corresponding States Principle and Related Topics

An equation of state (EOS) is a thermodynamic equation that describes a set of matter given a set of specific physical conditions, e.g., temperature, pressure, volume, enthalpy, or other state properties. These equations have been fields of study for researchers and scientists for a very long time. Among the earliest accepted equation of state is that proposed by van der Waals. It forms the basis for a theory called the principal of corresponding states, which is an extension of the van der Waals one-fluid model. The principal of corresponding states, hereafter CSP, is used to predict the state of a pure species or mixture based on the equation of state of a reference compound. The basic principle of CSP is that two fluids are in corresponding states if they are at the same reduced conditions, i.e., reduced temperature T_r and reduced volume V_r. There are several assumptions which must be made to utilize CSP, a hard sphere molecular model and similar energy states (Pitzner, 1939). The governing equation of CSP is shown in

Equation (1) below, where Z is traditionally the compressibility factor, but can represent any thermodynamic property, e.g., enthalpy, entropy, or internal energy. The superscript (0) indicates a conformal reference fluid.

$$Z(T_r, P_r) = Z^{(0)}(T_r, P_r) \quad (1)$$

The two most common implementations of CSP are multi-parameter CSP and generalized CSP. An excellent review of multi-parameter CSP was written by Leland and Chappelear (1968). Briefly, multi-parameter CSP uses empirical shape factors to correct for deviations from theory. Generalized CSP, hereafter GCSP, is championed by a series of authors who have built on the previous authors' work, the first of whom was Pitzner et al. (1955), then by Lee and Kessler (1975), followed by Teja et al. (1981), and most recently by Queimada et al. (2005). GCSP was selected for this study due to the lack of empirical parameters and the overall ease of implementation.

2.2.1 Generalized Corresponding States Principle

In theory, GCSP can be applied to any thermodynamic property and has also been extended to transport properties (Teja and Rice, 1981), but this work will focus on density and viscosity mixture predictions. A variety of investigative work has been previously done by various authors such as Teja et al (1981), Teja and Rice (1981 and 1981b), and by Queimada et al. (2005). Fundamental to GCSP is solution of the governing CSP equation by taking a Taylor series expansion about the reference fluid of the term, $Z^{(0)}$. In order for the expansion to be complete, the coefficients of the Taylor series must be obtained in such a way that the expansion is still fundamentally sound. The Pitzner acentric factor, ω, (Pitzner et al., 1995) is a measure of the deviation a molecule

has from a hard sphere, which, in light of the assumptions of CSP, makes the acentric factor a reasonable parameter to be used as the coefficient for the Taylor expansion. The acentric factor is defined in Equation (2) below:

$$\omega = -\log_{10}(P_r^{sat}) - 1 \quad \text{at} \quad T_r = 0.7 \tag{2}$$

For the generalized solution of Equation (1), Lee and Kessler used a single expansion and retained a hard sphere reference fluid (1975). The work conducted by Teja's group used are an expansion to the second term (see Equation (3)), meaning the working GCSP equation requires two reference fluids. The expansion used by Queimada (2005) is taken to the third term (see Equation (4)); therefore three reference fluids are required. The scripts (r#) indicate a reference fluid and X represents the property of interest.

$$X = X^{(r1)} + \frac{\omega - \omega^{(r1)}}{\omega^{(r2)} - \omega^{(r1)}}(X^{(r2)} - X^{(r1)}) \tag{3}$$

$$X = X^{(r1)} + \frac{X^{(r2)} - X^{(r1)}}{\omega^{(r2)} - \omega^{(r1)}}(\omega - \omega^{(r1)}) + \frac{\frac{X^{(r3)} - X^{(r1)}}{\omega^{(r3)} - \omega^{(r1)}} - \frac{X^{(r2)} - X^{(r1)}}{\omega^{(r2)} - \omega^{(r1)}}}{\omega^{(r3)} - \omega^{(r1)}}(\omega - \omega^{(r1)})(\omega - \omega^{(r2)}) \tag{4}$$

The authors of the papers mentioned above limited their work to pure components and relatively simple mixtures, such as binary or ternary mixtures, but implicit in the development of these equations is the ability to apply the equations to more complex mixtures (provided proper mixing rules are established). The ability of GCSP to address such complex mixtures is a significant portion of the work for this study.

2.2.2 Reference Fluids, Critical Properties, and Mixing Rules

An important part of understanding and applying GCSP is reference fluids and component information. Since jet fuels are such complex mixtures of hydrocarbons, the reference fluids must be similar in nature, i.e., a hydrocarbon fluid. The DIPPR 801

database, which is a chemical database maintained by the American Institute of Chemical Engineers (AIChE), provides an excellent source of expert-reviewed data on organic compounds. The database contains around 2000 unique compounds, of which around 300 of these components can be associated with jet fuel. Component information, i.e., T_c, V_c, MW, and ω, is also inherently important to the GCSP method. As such, obtaining information for the components used in the calculations is just as important. For this work, the two primary sources are the DIPPR 801 and a methodology introduced by Riazi and Daubert (1987). Furthermore, as mentioned previously, jet fuel is a mixture. Therefore, significant attention must also be paid to developing or selecting, and using appropriate mixing rules.

2.2.2.1 DIPPR 801 database

All of the reference fluids EOS and component properties used in this study were obtained from the DIPPR 801 database. The information that can be found includes critical properties and acentric factor, as well as more advanced correlations for liquid density and liquid viscosity. The DIPPR 801 database has established a standard set of equations that are used to calculate various chemical properties for a large number of organic compounds. For example, the functional form to relate liquid phase density (ρ) to temperature is:

$$\rho = \frac{A}{B^{\left[1+\left(1-\frac{T}{C}\right)^{D}\right]}} \tag{5}$$

Where, A, B, C and D, are coefficients determined by rigorous examination of all available literature data.

Table 1. Partial Table of Reference Fluids used for Liquid Density Calculations

Name	MW	T_c	V_c	ω	A	B	C	D
Ethane	30.06904	305.32	0.1455	0.099493	1.9122	0.27937	305.32	0.29187
n-Butane	58.1222	425.12	0.255	0.200164	1.0677	0.27188	425.12	0.28688
Isopentane	72.14878	460.4	0.306	0.227875	0.91991	0.27815	460.4	0.28667
1,1-dimethyl-cyclohexane	112.2126	591.15	0.45	0.232569	0.55873	0.25143	591.15	0.27758
Cumene	120.1916	631	0.434	0.327406	0.58711	0.25583	631	0.28494
n-propylbenzene	120.19	638.35	0.44	0.344391	0.57233	0.25171	638.35	0.29616
n-Nonane	128.2551	594.6	0.551	0.44346	0.46321	0.25444	594.6	0.28571
n-Decane	142.28	617.7	0.617	0.492328	0.41084	0.25175	617.7	0.28571

The equation of state used to calculate liquid viscosity with respect to temperature is:

$$\eta = e^{\left[A+\frac{B}{T}+C*\ln T+ D*T^E\right]} \quad (6)$$

Where, again, *A*, *B*, *C* and *D*, are coefficients derived from a critical evaluation of all available data. The coefficients for a partial list of the selected reference fluids are shown in Table 1 and Table 2. The two tables list the coefficients used in Equations (5) and (6), respectively, for the selected reference fluids, of which more complete tables can be found in Appendix A.2, p. A.8.

Table 2. Partial Table of Reference Fluids used for Liquid Viscosity Calculations

Name	MW	T_c	V_c	ω	A	B	C	D	E
Isooctane	114.2285	543.8	0.468	0.303455	-11.432	1074	0.015358	0	0
Cumene	120.1916	631	0.434	0.327406	-11.756	1483.1	-0.04039	0	0
n-Propylbenzene	120.1916	638.35	0.44	0.344391	-18.282	1549.7	1.0454	0	0
n-Butylbenzene	134.2182	660.5	0.497	0.394149	-11.273	1528.8	-0.10761	0	0
n-Tridecane	184.3614	675	0.826	0.617397	-111.98	5468.6	15.579	-1.7E-05	2
n-Tetradecane	198.388	693	0.897	0.643017	-136.73	6421.3	19.493	-2.3E-05	2

2.2.2.2 Riazi and Daubert Component Estimation

When critical property data is unknown, for instance, multi-component hydrocarbon fractions, estimation techniques are required. Riazi (2005) has written extensively regarding the estimation of critical properties for hydrocarbons and hydrocarbon fractions. For hydrocarbon systems, the most important intermolecular force is London's dispersion forces. It follows that the potential energy function, for non-polar molecules that abide by the Mie relation, can be represented by the well-known Leonard-Jones potential. This two-parameter function represents the potential energy function in terms of a molecular energy parameter and a molecular size parameter. Riazi and Daubert (1987) showed that these two parameters can be subsequently represented by readily available, related quantities, such as the boiling temperature, T_b, and specific gravity, SG, of a substance. Furthermore, they developed a series of equations, more specifically one equation with different coefficients, to estimate the critical properties of hydrocarbons based on various parameter pairs. This equation estimates a property of interest based upon known properties.

$$\theta = a \cdot \exp(b\theta_1 + c\theta_1 + d\theta_1\theta_2) \cdot \theta_1^e \theta_2^f \tag{7}$$

In Equation (7), θ represents the property of interest, for example, critical temperature, θ_1 and θ_2 represent known properties, such as molecular weight and carbon-to-hydrogen ratio, and the letters *a* to *f* represent coefficients found by the work done by Riazi and Daubert (1987). The second estimation that Riazi presents is various methods for estimating the acentric factor of hydrocarbons. From among the various methods Riazi presented, a method described by Lee and Kessler (1975) was selected.

$$\omega_{L-K} = \frac{\frac{-\ln P_c}{1.01325} - 5.92714 + \frac{6.09648}{T_{br}} + 1.28862 \cdot \ln T_{br} - 0.169347 \cdot T_{br}^6}{15.2518 - \frac{15.6875}{T_{br}} - 13.4721 \cdot \ln T_{br} + 0.43577 \cdot T_{br}^6} \quad (8)$$

Where, T_{br} represents the reduced boiling point ($T_{br} = T_b/T_c$) and P_c represents the critical pressure.

2.2.2.3 Mixing Rules

It follows from the van der Waals one-fluid model that the mixture is treated as a pure component. As such, the critical properties of the mixture must be evaluated. These properties are often estimated using mixing rules, as evaluating the critical properties of a mixture is an extremely difficult experimental process. Using mixing rules results in the usage of pseudo-critical mixture properties for temperature, T_{cm}, and volume, V_{cm}, which are well represented by components of the mixture. Selection of appropriate mixing rules is nontrivial; however, most of those used for hydrocarbon mixtures are again based on London's dispersion forces since these mixtures are non-polar and non-associating. Starting with the simplest and going to the most complex: molecular weight, acentric factor, critical volume, and critical temperature are all necessary for the implementation of GCSP for mixtures. The mixing rule used for molecular weight is a simple mole fraction weighted average, i.e., Kay's rule as shown in Equation (9) below, where x_i is the mole fraction of the i^{th} species, MW_i is the molecular weight of the i^{th} species, and n is the total number of mixture components,

$$MW_{mix} = \sum_{i=1}^{n} x_i MW_i \quad (9)$$

Kay's rule is also used for calculation of acentric factor.

$$\omega_{mix} = \sum_{i=1}^{n} x_i \omega_i \tag{10}$$

There are several different ways to calculate the pseudo-critical properties of a mixture, one of which is represented by Teja and Rice (1981).

$$V_{cm} = \sum\sum_{ij} x_i x_j V_{c,ij} \tag{11}$$

Where,

$$V_{c,ij} = \frac{\left(V_{c,ii}^{1/3} + V_{c,jj}^{1/3}\right)^3}{8} \tag{12}$$

This formula for the pseudo-critical volume is dependent on the mixture components. But, the formula also ensures that when $i = j$, the value of $V_{c,ij}$ is the value of the pure component species i. Pseudo-critical temperature can be represented by:

$$T_{cm} = \frac{\sum\sum_{ij} x_i x_j T_{c,ij} V_{c,ij}}{V_{cm}} \tag{13}$$

Where,

$$T_{c,ij} V_{c,ij} = \alpha_{ij} \sqrt{T_{c,ii} V_{c,ii} T_{c,jj} V_{c,jj}} \tag{14}$$

In Equation (14) the α_{ij} represents the binary interaction coefficient. This coefficient represents the molecular interactions between two different chemical species. Thus when the value of α_{ij} is one, it represents an ideal mixture. There are two ways to approach this term for non-ideal mixtures. Teja (1981, 1981b) and Queimada (2005) approach this value empirically. They did this by regressing values for α_{ij} from large amounts of experimental data. The theoretical basis for this coefficient is based on London's dispersion forces. One solution of these interactions is shown in Equation (15) below and is from Prausnitz (1967):

$$\alpha_{ij} = \left[\frac{\sqrt{V_{c,i}^{1/3} V_{c,j}^{1/3}}}{\frac{\left(V_{c,i}^{1/3} + V_{c,j}^{1/3}\right)}{2}}\right]^3 \quad (15)$$

As can be seen, this version of the binary interaction calculation is strictly a function of the pure component critical volumes.

2.3 Objective

The goal of this study will be multi-part, first and foremost, to prove that GCSP is usable for complex mixtures. Use this proof to apply GCSP to a thermodynamic property of jet fuel, e.g., density, and on a transport property, e.g., viscosity. These aspects combined will be the overall objective of this study as well as to further the field of GCSP by proving the usefulness of the technique to complex mixtures.

CHAPTER 3

METHODS

Several calculations were required prior to operating the actual GCSP method. This was due to the simplifications of the complex fuel composition. Each compositional group needed to have critical properties assigned, which was straightforward for pure components, but required estimation techniques for the pseudo-groups. There were three methods for accomplishing these estimations. The first method was to use regression from existing data values for each compositional group. The second method was to use the calculation introduced by Riazi and Daubert (1987) for hydrocarbon fractions to estimate the critical properties. The third method was a hybrid of the first two methods. The differences in these methods are enough to significantly change the results, and as such, are discussed with more depth in the results.

3.1 GCSP Method

First, data compositional information about a sample is obtained via GCxGC measurement. GCxGC data is recorded as a relative mass response, which is directly proportional to the mass fraction of carbon and can be converted into mole fractions.

Conversion to mole fraction of compound *i* is illustrated in Equations (16) and (17) below. Equation (16) yields the mass of the pseudo-group, and equation (17) converts that information to a mole fraction. In these equations, the subscript 'i' indicates the pseudo-group of which the mole fraction is being calculated and CN represents the carbon number of the group.

$$w_i = \frac{GC \cdot MW_i}{MW_{carbon} \cdot CN_i} \tag{16}$$

$$x_i = \frac{w_i}{MW_i \sum w_i} \tag{17}$$

Mixture physical and pseudo-critical properties, i.e., MW_m, ω_m, T_{cm}, and V_{cm}, were obtained by applying Equations (9) to (14), with $\alpha_{ij} = 1$, using the following procedure: (i) Determine the temperature, T, at which to estimate the property of interest, (ii) Use this temperature, T, with the pseudo-critical temperature, T_{cm}, to calculate the reduced temperature, $T_r = T/T_{cm}$, (iii) Use the EOS for the reference fluids (see Section 2.2.2.1) to evaluate the value of the reference fluid properties at determined T_r, (iv) Apply the values obtained from (iii) inside of the GCSP equation for the property of interest, and use equation (19), (20), or (24) to predict the desired property of the mixture. The equations for the properties calculated in this work can be found in the sections below, titled respectively density and viscosity.

3.1.1 Density

The existing literature has equations for predicting the specific volume from which density can be obtained. The equation that is found in literature (Teja et al., 1981) is:

$$\frac{v_m}{V_{cm}} = \frac{v^{(r1)}}{V_c^{(r1)}} + \frac{\omega_m - \omega^{(r1)}}{\omega^{(r2)} - \omega^{(r1)}}\left(\frac{v^{(r2)}}{V_c^{(r2)}} - \frac{v^{(r1)}}{V_c^{(r1)}}\right) \tag{18}$$

Where, v is specific volume, V is critical volume, and ω is the acentric factor. This equation can be modified to calculate density. The modifications, which include converting for desired units (g/cm^3), change the equation for the two-parameter GCSP from equation (18) above to equation (19) below:

$$\rho_m = \left(\frac{MW_m}{10^3}\right)\left[V_{cm}\left(\frac{\frac{1}{\rho^{(r1)}}}{V_c^{(r1)}} + \frac{\omega_m - \omega^{(r1)}}{\omega^{(r2)} - \omega^{(r1)}}\left(\frac{\frac{1}{\rho^{(r2)}}}{V_c^{(r2)}} - \frac{\frac{1}{\rho^{(r1)}}}{V_c^{(r1)}}\right)\right)\right]^{-1} \tag{19}$$

Or for the three-parameter GCSP, the equation is:

$$\rho_m = \left(\frac{MW_m}{10^3}\right)\left[V_{cm}\left(\frac{\frac{1}{\rho^{(r1)}}}{V_c^{(r1)}} + D_1\left(\omega_m - \omega^{(r1)}\right) + D_2\left(\omega_m - \omega^{(r1)}\right)\left(\omega_m - \omega^{(r2)}\right)\right)\right]^{-1} \tag{20}$$

Where,

$$D_1 = \frac{\left(\frac{\frac{1}{\rho^{(r2)}}}{V_c^{(r2)}} - \frac{\frac{1}{\rho^{(r1)}}}{V_c^{(r1)}}\right)}{\left(\omega^{(r2)} - \omega^{(r1)}\right)} \tag{21}$$

And,

$$D_2 = \frac{\frac{\left(\frac{\frac{1}{\rho^{(r3)}}}{V_c^{(r3)}} - \frac{\frac{1}{\rho^{(r1)}}}{V_c^{(r1)}}\right)}{\left(\omega^{(r3)} - \omega^{(r1)}\right)} - D_1}{\omega^{(r3)} - \omega^{(r1)}} \tag{22}$$

Equations (19) and (20) are the equations that are used in the model to predict density in this work.

3.1.2 Viscosity

Viscosity is not a true thermodynamic variable, but rather a transport variable. It is experimentally difficult to obtain a critical viscosity, and therefore, an alternative reducing factor for viscosity is required for GCSP. As such, the equations in literature (Teja and Rice, 1981) developed a pseudo-reducing factor that is based on theory. The reducing factor is shown below:

$$\xi = \frac{V_c^{2/3}}{T_c^{1/2} MW^{1/2}} \tag{23}$$

Thus the workable form of the GCSP expression becomes equation (24) and is written below (Teja and Rice, 1981):

$$\ln(\eta\xi) = \ln(\eta\xi)^{(r1)} + \frac{\omega - \omega^{(r1)}}{\omega^{(r2)} - \omega^{(r1)}}\left[\ln(\eta\xi)^{(r2)} - \ln(\eta\xi)^{(r1)}\right] \tag{24}$$

Where, η stands for viscosity, ξ is the reducing factor mentioned above (equation (23)), and ω is the acentric factor. The form is identical to the equations used in the density predictions except with respect to the reducing factor and is applied to different properties. Equation (24) above is rearranged into the more functional form shown in equation (25) below:

$$\eta = \frac{(\eta\xi)_{(r2)}^{\left(\frac{\omega-\omega^{(r1)}}{\omega^{(r2)}-\omega^{(r1)}}\right)} (\eta\xi)_{(r1)}^{\left(1-\left(\frac{\omega-\omega^{(r1)}}{\omega^{(r2)}-\omega^{(r1)}}\right)\right)}}{\xi} \tag{25}$$

3.1.3 Error Measurement

Two measurement metrics were used to assess the data: the average absolute deviation (AAD%) and the average error at a nominal temperature (zone error%). For density, the

actual temperatures are about +/- 1°C of the following nominal temperatures; -35.5, -19, -0.2, 20, 39.5, 68.7 °C. For viscosity, the nominal temperatures are -40, -20, and 20 °C and are the actual temperatures. The average absolute deviation, equation (29), was taken as a function of the point error, equation (26), of each data point in order to build a uniform measurement system across multiple data sets. The average error percent, equation (27), is representative of the bias. The AAD% is a measure of the models' precision.

$$y_i = \left(\frac{Experimental_i - Model_i}{Model_i}\right) \cdot 100 = Point\ Error\ Percent \tag{26}$$

$$Total\ Average\ Error\ Percent = \frac{\sum_i y_i}{n} = Ave\% \tag{27}$$

$$Zone\ Error\ Percent = \frac{\sum_c y_i}{c} \tag{28}$$

$$AAD\% = \frac{1}{n}\sum_n |y_i - Ave\%| \tag{29}$$

Where, subscript *i* indicates an individual data point, c indicates the number of points at a nominal temperature, i.e., the total number of fuels, and *n* indicates the total number of data points.

CHAPTER 4

RESULTS AND DISCUSSIONS

It is desirable to develop models to predict jet fuel properties based on mixture component concentrations. As mentioned previously in the background information, there are multiple CSP techniques to do so; however, this work will explore the use of GCSP. This method was selected due to its ease of use and success in the literature for prediction of pure compounds and simple (binary and tertiary) mixtures (Teja and Rice, 1981, 1981b, Queimada et al., 2005).

4.1 Density

4.1.1 Pseudo-Groups

One major problem with direct implementation of GCSP to jet fuel is the complexity of the fuel. Jet fuel is composed of thousands of hydrocarbons, and quantification of each component is impractical. Surrogate mixtures are often used during experimentation; however, this is inappropriate for predictive modeling. For both computational and practical purposes, simplification of the fuel was done by lumping similar chemicals into

distinct groups based on carbon number and hydrocarbon type. An example group is C_8H_{10}, which is the molecular formula for four isomers; ethyl-benzene and the three variations of xylene. Obviously, as the number of carbons increase the number of distinct isomers increases. As such, a method is necessary to calculate or obtain pseudo-critical information for these components from a potentially small selection of molecules. The total concentration of the smaller or larger molecules is very small in comparison to the listed molecular group. Table 3 shows the group names, molecular formulas, and lists some examples of isomer counts for the components that will be used later. In Table 3, there are highlighted plus and minus symbols. These groups include molecules that are smaller or larger than the listed carbon number, depending on the respective symbol. This grouping happens due to chromatography and concentration limits, i.e., the total concentration of the smaller or larger molecules is very small in comparison to the listed molecular group.

Table 3. Group Names, Molecular Formulas, and Isomer Count Examples

Name	Molecular formula	# of Isomers	Name	Molecular formula	# of Isomers	Name	Molecular formula	# of Isomers
C_{00}-benzene	C_6H_6	1	dicyclo-C_{13}	$C_{13}H_{24}$		monocyclo-C_{12}	$C_{12}H_{24}$	
C_{01}-benzene	C_7H_8	1	dicyclo-C_{14}	$C_{14}H_{26}$		monocyclo-C_{13}	$C_{13}H_{26}$	
C_{02}-benzene	C_8H_{10}	4	dicyclo-C_{15}	$C_{15}H_{28}$		monocyclo-C_{14}	$C_{14}H_{28}$	
C_{03}-benzene	C_9H_{12}	8	dicyclo-C_{16}	$C_{16}H_{30}$		monocyclo-C_{15}	$C_{15}H_{30}$	
C_{04}-benzene	$C_{10}H_{14}$	22	dicyclo-C_{17}+	$C_{17}H_{32}$		monocyclo-C_{16}	$C_{16}H_{32}$	
C_{05}-benzene	$C_{11}H_{16}$	40	iso-C_{07}-	C_7H_{16}	9	monocyclo-C_{17}	$C_{17}H_{34}$	
C_{06}-benzene	$C_{12}H_{18}$	87	iso-C_{08}	C_8H_{18}	18	monocyclo-C_{18}	$C_{18}H_{36}$	
C_{07}-benzene	$C_{13}H_{20}$		iso-C_{09}	C_9H_{20}	35	monocyclo-C_{19}+	$C_{19}H_{38}$	
C_{08}-benzene	$C_{14}H_{22}$		iso-C_{10}	$C_{10}H_{22}$	75	n-C_{07}	C_7H_{16}	1
C_{09}-benzene	$C_{15}H_{24}$		iso-C11	$C_{11}H_{24}$	159	n-C_{08}	C_8H_{18}	1
C_{10}- benzene+	$C_{16}H_{26}$		iso-C12	$C_{12}H_{26}$	355	n-C_{09}	C_9H_{20}	1
cycloaromatic-C_{09}	C_9H_{10}		iso-C13	$C_{13}H_{28}$	802	n-C_{10}	$C_{10}H_{22}$	1
cycloaromatic-C_{10}	$C_{10}H_{12}$		iso-C14	$C_{14}H_{30}$	1,858	n-C_{11}	$C_{11}H_{24}$	1
cycloaromatic-C_{11}	$C_{11}H_{14}$		iso-C15	$C_{15}H_{32}$	4,347	n-C_{12}	$C_{12}H_{26}$	1
cycloaromatic-C_{12}	$C_{12}H_{16}$		iso-C16	$C_{16}H_{34}$	10,359	n-C_{13}	$C_{13}H_{28}$	1
cycloaromatic-C_{13}	$C_{13}H_{18}$		iso-C17	$C_{17}H_{36}$	24,894	n-C_{14}	$C_{14}H_{30}$	1
cycloaromatic-C_{14}	$C_{14}H_{20}$		iso-C18	$C_{18}H_{38}$	60,523	n-C_{15}	$C_{15}H_{32}$	1
cycloaromatic-C_{15}+	$C_{16}H_{24}$		iso-C19	$C_{19}H_{40}$	148,284	n-C_{16}	$C_{16}H_{34}$	1
diaromatic-C_{10}	$C_{10}H_8$		iso-C20	$C_{20}H_{42}$	366,319	n-C_{17}	$C_{17}H_{36}$	1
diaromatic-C_{11}	$C_{11}H_{10}$		iso-C21	$C_{21}H_{44}$	910,726	n-C_{18}	$C_{18}H_{38}$	1
diaromatic-C_{12}	$C_{12}H_{12}$		iso-C22	$C_{22}H_{46}$	2,278,658	n-C_{19}	$C_{19}H_{40}$	1
diaromatic-C_{13}	$C_{13}H_{14}$		iso-C23	$C_{23}H_{48}$	5,731,580	n-C_{20}	$C_{20}H_{42}$	1
diaromatic-C_{14}+	$C_{14}H_{16}$		iso-C24+	$C_{24}H_{50}$	14,490,245	n-C_{21}	$C_{21}H_{44}$	1
dicyclo-C_{08}	C_8H_{14}		monocyclo-C07-	C_7H_{14}		n-C_{22}	$C_{22}H_{46}$	1
dicyclo-C_{09}	C_9H_{16}		monocyclo-C08	C_8H_{16}		n-C_{23}	$C_{23}H_{48}$	1
dicyclo-C_{10}	$C_{10}H_{18}$		monocyclo-C09	C_9H_{18}		tricyclo-C_{10}	$C_{10}H_{16}$	
dicyclo-C_{11}	$C_{11}H_{20}$		monocyclo-C10	$C_{10}H_{20}$		tricyclo-C_{11}	$C_{11}H_{18}$	
dicyclo-C_{12}	$C_{12}H_{22}$		monocyclo-C11	$C_{11}H_{22}$		tricyclo-C_{12}	$C_{12}H_{20}$	

As can be seen in Table 3 above, the number of isomers grows exponentially for a given homologous series with the exception of normal alkanes. In particular, the iso-paraffin group that contains twenty-four carbons (highlighted) is a prime example of the extensive number of isomers that can occur. In order to obtain the properties for these groups, three methods were utilized to group the components to be represented by a single pseudo-component. The first is a numerical method using existing data for multiple species within a homologous series to regress a given property. The second method is a theoretical based calculation selected from a variety of options presented by Riazi (2005)

which attempts to calculate the needed information from known properties, such as molecular weight or carbon-to-hydrogen ratio. The third method was a combination of the previous two methods. It should be noted that for all of these methods, if a single isomer occurs for a group, the database (DIPPR 801) information was used for it, e.g., benzene, toluene, naphthalene, and the normal paraffins. In order to effectively compare each of these methods, a standard pair of reference fluids was selected for use, but these may not be the optimum selection (see the Reference Fluids section beginning on p. 30). The two reference fluids were n-propylbenzene and n-decane.

4.1.1.1 Method 1 – Numerical Regression for Critical Property Estimates

One method to obtain critical property data for the pseudo-groups is a numeric regression of data points for different species within a class obtained from the DIPPR 801 database. The list of species used to obtain these regressions is found in Appendix A. Figure 2 below is a sample regression of the critical volume for the alkyl-benzene family. The regression is a function of carbon number, (CN). Carbon number was selected to be the independent variable because it allows for reducing the number of points from the database, as well as to extrapolate points where the database is lacking information.

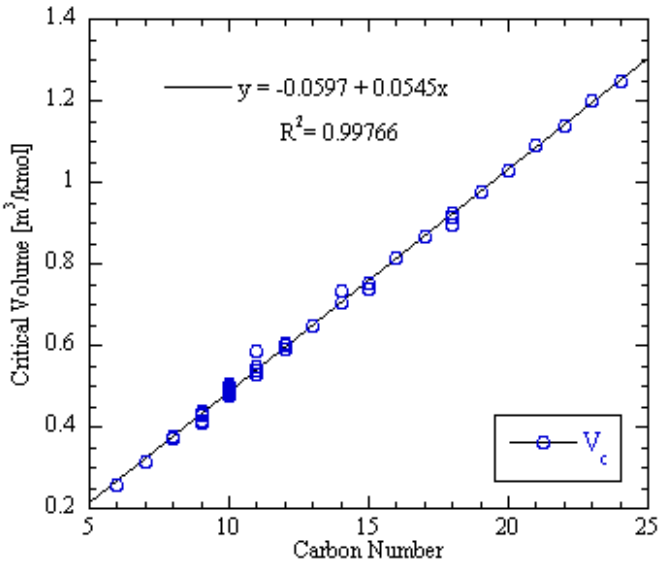

Figure 2. Plot of critical volume vs. carbon number for alkyl-benzenes pseudo-group.

Table 4 lists the equations that were used to calculate the information for the pseudo-groups. It should be noted that the cyclo-aromatic group and the tri-cyclo-paraffin groups' critical temperature is a different functional form from the other sets. This is a direct result of the available data for these groups, which is a known deficit of the methodology.

Table 4. Regression Equations

Family	T_c [K]	V_c [m^3/kmol]	Acentric Factor
Alkyl-Benzene	$T_c = 217.49 \cdot \ln CN + 120.41$	$V_c = 0.0545 \cdot CN - 0.0597$	$\omega = 0.0414 \cdot CN - 0.0281$
Cyclo-Aromatic	$T_c = 12.208 \cdot CN + 585.362$	$V_c = 0.056 \cdot CN - 0.1236$	$\omega = 0.0408 \cdot CN - 0.0643$
Di-aromatic	$T_c = 150.47 \cdot \ln CN + 619.47$	$V_c = 0.0503 \cdot CN - 0.082$	$\omega = 0.0347 \cdot CN - 0.0061$
Di-cyclo-paraffin	$T_c = 260.15 \cdot \ln CN + 88.987$	$V_c = 0.0473 \cdot CN + 0.0184$	$\omega = 0.0512 \cdot CN - 0.2064$
Iso-paraffin	$T_c = 222.49 \cdot \ln CN + 97.591$	$V_c = 0.0533 \cdot CN + 0.0387$	$\omega = 0.0297 \cdot CN + 0.0995$
Cyclo-paraffin	$T_c = 209.37 \cdot \ln CN + 161.89$	$V_c = 0.0534 \cdot CN - 0.0015$	$\omega = 0.0374 \cdot CN - 0.0175$
n-paraffin	All values come from tabulated DIPPR 801 data.		
Tri-cyclo-paraffin	$T_c = 2.5 \cdot CN + 678$	$V_c = 0.0425 \cdot CN + 0.06$	$\omega = 0.0541 \cdot CN - 0.3557$

The complete table of numerical values can be found in Appendix B.1. The appendix also lists whether the values are database or regression values, i.e., generally indicates whether a substance has a single isomer. Having established a method to estimate critical

properties and acentric factor for the pseudo-groups, these values were used in the GCSP algorithm to compute density. Figure 3 shows the results of the computation for three fuel samples: a JP-8 (F3896), Jet A (F3962), and a Jet A-1 (F4158); the markers are experimental CRC data and the lines are the predictions.

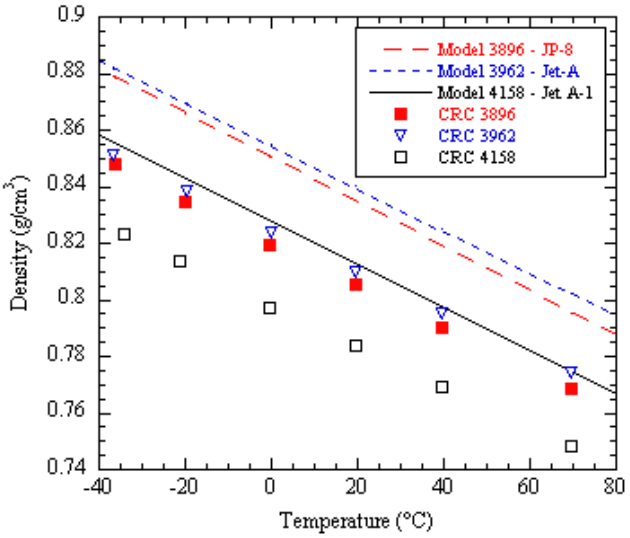

Figure 3. Density profiles of three fuel samples; markers are experimental data (CRC) and lines are predictions using Method 1 for critical property estimates.

The figure shows that the model overestimates the density for all three fuel samples. Regardless of the bias, the predicted slopes of the density with respect to temperature are well matched to the data. The same method was applied to the entire data set of about 310 data points (52 fuels with 6 temperatures per fuel) and the predicted results are shown versus the experimental data in Figure 4 below. In all of the parity plot figures, the solid blue line indicates x = y or the 1-to-1 line, and the dashed ±2.5% lines are shown for reference. The average overestimation for the entire data set was about 3.20% (average error mentioned in the section 3.1.3), at all temperatures. The slope of the data is near to unity. The average absolute deviation (AAD%) of the data set is 0.24%, which indicates

the data has low variation from the average bias. Therefore, it is worthwhile to further investigate this property prediction method.

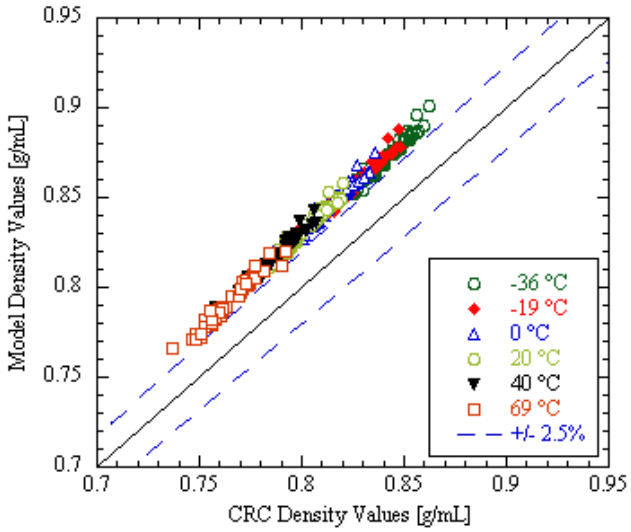

Figure 4. Full data set plot of the predicted values versus experimental values using Method 1 critical property estimations.

4.1.1.2 Method 2 – Semi-Theoretical Estimation of Critical Properties

The second method of obtaining the values for the component groups is from Riazi and Daubert (1987). This method is a semi-theoretical technique that was developed to predict the properties of hydrocarbons. Table 5 below lists the coefficients used in equation (7) (see section 2.2.2.2) to calculate the desired property. It should also be noted that in order to calculate the acentric factor, equation (8), critical pressure and boiling point must also be calculated.

Table 5. Coefficients for Estimation of Critical Properties of Pseudo-Groups (Riazi and Daubert, 1987)

Property	θ_1	θ_2	a	b	c	d	e	f
T_c	MW	CH	20.74	$1.385 \cdot 10^{-3}$	-0.1379	$-2.7 \cdot 10^{-4}$	0.3526	1.4191
V_c	MW	CH	$1.597 \cdot 10^{1}$	$-2.3533 \cdot 10^{-3}$	0.1082	$3.826 \cdot 10^{-4}$	0.0709	-1.3362
P_c	MW	CH	56.26043	$-2.139 \cdot 10^{-3}$	-0.265	0	-0.6616	2.4004
T_b	MW	CH	20.25347	$-1.57415 \cdot 10^{-4}$	$-4.5707 \cdot 10^{-2}$	$9.22926 \cdot 10^{-6}$	0.512976	0.472372

With the pseudo-groups calculated, the GCSP method was applied to the data set, i.e., the only factor that had changed from Section 4.1.1.1 is the pseudo-group information. This yielded Figure 5 (below) which shows the computation for three fuel samples: a JP-8 (F3896), Jet A (F3962), and a Jet A-1 (F4158); the markers are experimental CRC data and the lines are the predictions. Again, the model overestimates each of the fuels by a few percent. Despite the bias, the predicted slopes of the density with respect to temperature are well matched to the data.

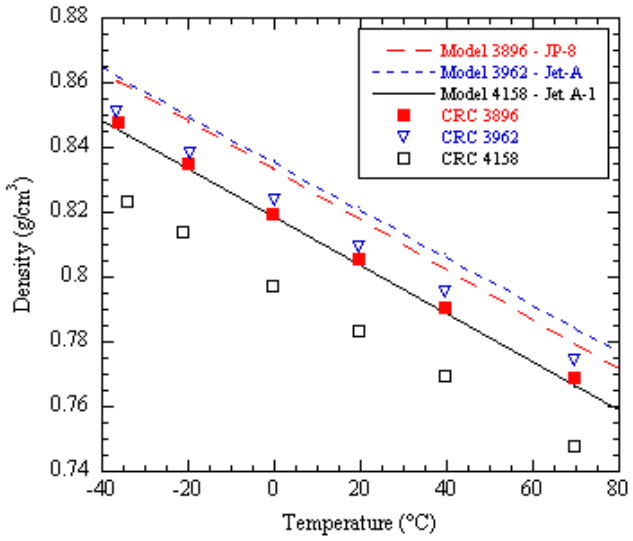

Figure 5. Density profiles of three fuel samples; markers are experimental data (CRC) and lines are predictions using Method 2 for critical property estimates.

The same method was applied to the entire data set and the predicted results are shown versus the experimental data in Figure 6 below. The average overestimation for the entire

data set was about 1.46% at all temperatures. Furthermore, the data tends to display isotherms inside of the data. These isotherms tend to broaden the uncertainty of the overall correlation, i.e., the predictions are less precise. These isotherms result in a higher AAD of 0.65%.

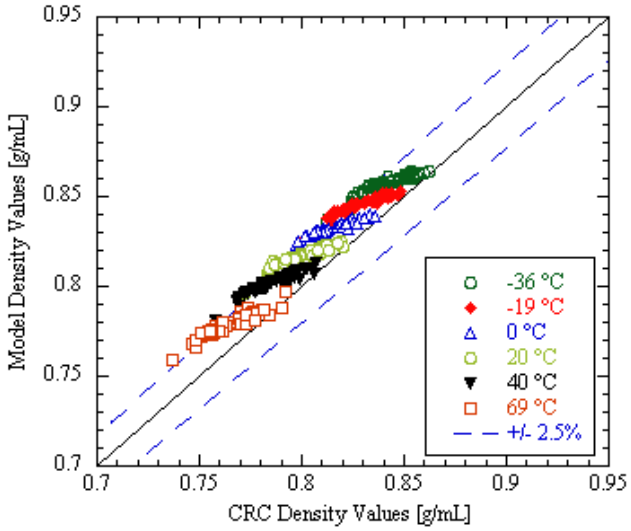

Figure 6. Full data set plot of the predicted values versus experimental values using Method 2 critical property estimations.

4.1.1.3 Method 3 – Hybrid Estimation of Critical Properties

The final method used to estimate critical properties for pseudo-groups is a combination of both the Riazi/Daubert and the numerical regression. This hybrid method was attempted in order to more thoroughly investigate the way that pseudo-groups were calculated. The method was constructed by using the pure component data for compounds that had a single isomer, e.g., n-paraffins, benzene, toluene, and naphthalene. Since this method was exploratory, it was decided to use the regression groups for the following families of substances: cyclo-aromatics, di-aromatics, and di-cyclo-paraffins.

The Riazi/Daubert method was used for the remaining families, i.e., alkyl-benzenes, mono-cyclo-paraffins, tri-cyclo-paraffins, and iso-paraffins. This method had some distinct differences from methods of which it is comprised. These factors are demonstrated in the following two figures below (Figure 7 and Figure 8). Figure 7 shows the strong slope similarities in the lines of the model, i.e., the lines have a slope that matches the slope of a line drawn through the experimental points. Figure 8 demonstrates the average error and high spread of this method. The average error for the data set is 3.17%, which is comparable to method 1 in magnitude but not in bias. However, the AAD% is much higher than either of the previous models at 1.90%. So while the error of the hybrid method is comparable to the first two methods, the precision of method 3 is poor.

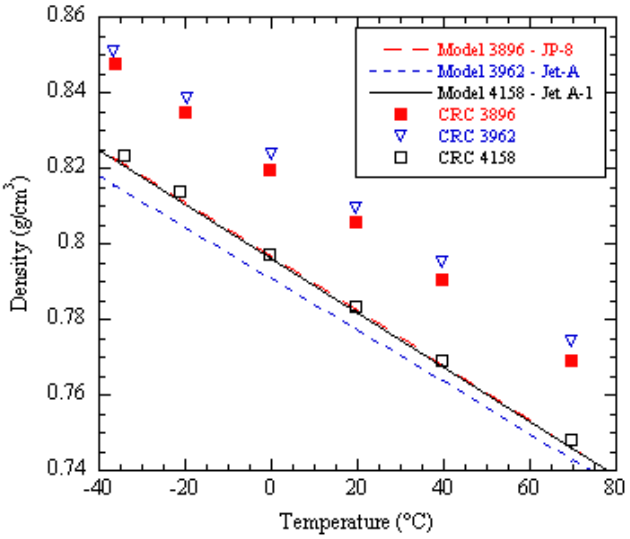

Figure 7. Density profiles of three fuel samples; markers are experimental data (CRC) and lines are predictions using Method 3 for critical property estimates.

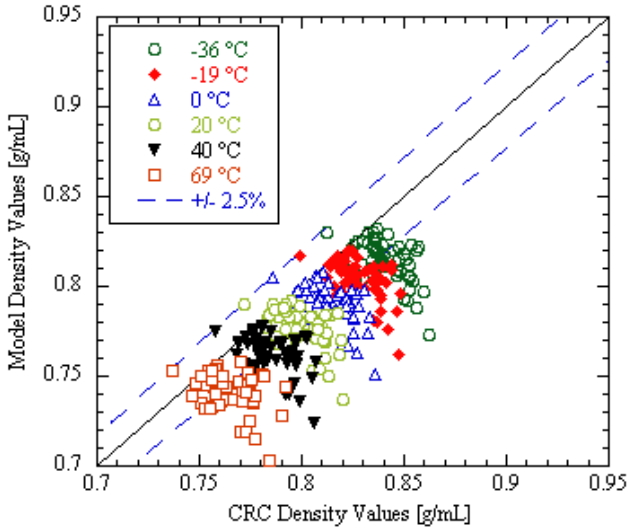

Figure 8. Full data set plot of the predicted values (y-axis) versus experimental values (x-axis) using Method 3 critical property estimations.

4.1.1.4 Summary of Critical Property Estimation for Pseudo-Groups

In summary, pseudo-groups and the method that is used to obtain the critical properties of the said pseudo-groups are important factors of GCSP. This is self-evident as varying the method of pseudo-critical calculation drastically changes the outcome of the model. But out of these three methods, it is suggested that either method 1 or method 2 be selected when using n-propylbenzene and n-decane as reference fluids. This is recommended due to the low AAD% and average percent error as seen in Table 6 below.

Table 6. Statistics from n-propylbenzene/n-decane reference fluids

Method	Reference Fluid #1	Reference Fluid #2	AAD%	Ave%
Numerical Regression	n-propylbenzene	n-decane	0.25	-3.20
Riazi/Daubert	n-propylbenzene	n-decane	0.65	-1.46
Hybrid	n-propylbenzene	n-decane	1.90	3.17

The following section will address the impact of reference fluid selection on the outcome of the model.

4.1.2 Examining Reference Fluids

Selection of reference fluids is an important factor in modelling with GCSP. The following section will examine and evaluate the importance and sensitivity that the references fluids have on the model. In order to search for the 'optimum' reference fluids, an algorithm was designed. This algorithm uses the information from the DIPPR database to obtain pairs of reference fluids that minimized the value of Δ. Δ (equation (30) below) is the product of the absolute value of the zone error, i.e., the nominal temperature error (Equation (28)), and absolute average deviation (equation (29)).

$$\Delta = |Zone\ Err\% \cdot AAD\%| \tag{30}$$

Zone error is used here as it is able to account for the error at each nominal temperature, as well as any switches from positive error to negative error or vice versa, i.e., the data starts on one side of the 1-to-1 line at one temperature zone and is on the other side of the line for the next temperature zone. This transition effectively zeroes the average error. As this phenomenon can also occur within a nominal temperature region, the algorithm uses zones to minimize the impacts of these transitions. In order to sort the algorithm output, each pair of reference fluids was assigned a number so that the results obtained from the algorithm could be sorted and applied effectively. The pairs obtained from this procedure are optimal for the critical property calculation method, and exclusively that method. The algorithm was applied to the three methods for critical property estimation. This resulted in a set of statistics and optimum pairs for all three of the property estimation methods.

The optimums for each method are listed in Table 7 below. From this data, the hybrid method results in the lowest Δ, but it also has the highest variability (AAD%). The Numerical Regression method has the lowest variability. Further analysis is needed to distinguish between these methods and their suitability to the goal of this work.

Table 7. Optimum Results from Algorithm for Each Critical Property Estimation Method

Method	Reference Fluid #1	Reference Fluid #2	Zone Err%	AAD%	Δ	Ave%
Numerical Regression	Ethane	Isopentane	-0.023	0.225	0.0045	-0.0078
Riazi/Daubert	1,1-dimethyl-cyclohexane	n-nonane	0.010	0.97	0.0097	-0.10
Hybrid	n-butane	Cumene	0.0025	1.84	0.0046	0.0035

As can be seen by comparing Table 6 and Table 7, there is improvement in the average error of all three critical property estimation techniques that comes from optimizing the reference fluids, decreasing by at least 1.25% across all three methods. However, the AAD% is, in general, not drastically improved. To further analyze the information obtained from the algorithm, each of the optimum pairs was plotted on a parity plot against the experimental data. Figure 9, the numerical regression critical property method, displays a compact grouping of data that is tightly grouped along the one-to-one line. The centering along the one-to-one line is common among all three methods, a result of the low average error of each method. But, Figure 10, which displays the Riazi/Daubert method, and Figure 11, which illustrates the hybrid method, are less compact, a reflection of their higher AAD%. Another thing to note about Figure 10 is the isotherms that appear in the predicted data. By interpreting both the figures and the data in Table 7, it becomes obvious that the numerical regression method, with its optimum reference fluids, produces the most accurate results.

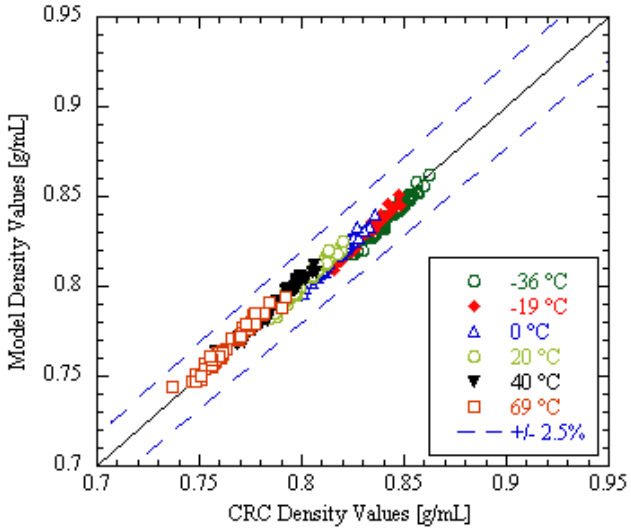

Figure 9. Parity plot with numerical regression critical property estimates using the optimum fluids, ethane and isopentane.

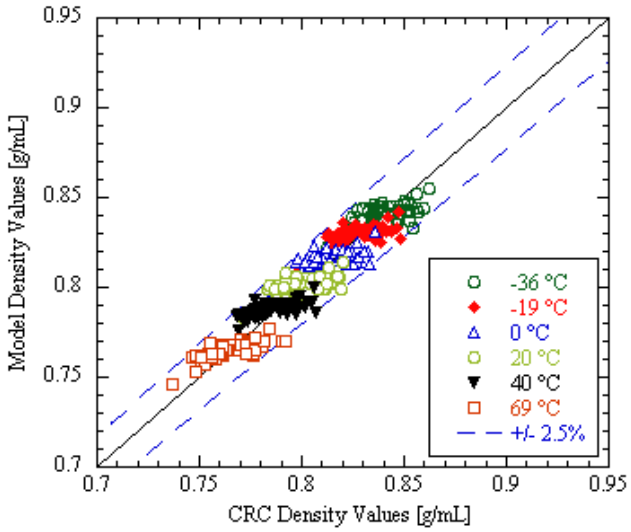

Figure 10. Parity plot with Riazi/Daubert critical property estimates using the optimum fluids, 1,1-dimethylcyclohexane and n-nonane.

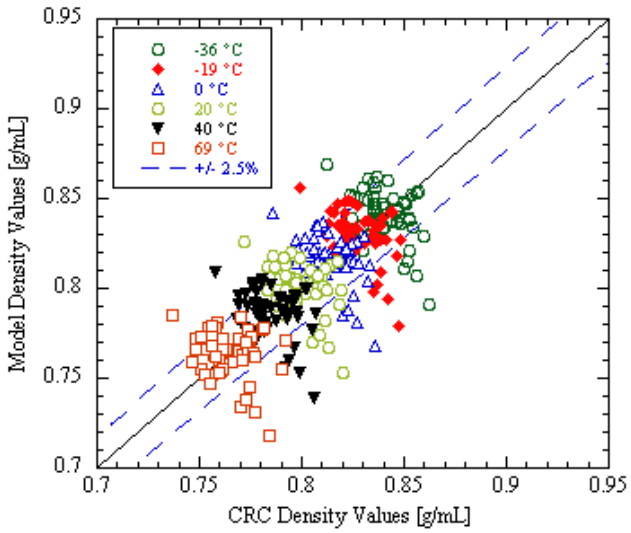

Figure 11. Parity plot with hybrid critical property estimates using the optimum fluids, n-butane and cumene.

4.1.2.1 Importance of Optimum Reference Fluids

From Table 7, the regression-based pseudo-groups have the optimum reference fluids of ethane and isopentane. For explorative purposes, this pair of reference fluids was applied to each critical property estimation method and comparatively analyzed. When these reference fluids are applied to the system with the various pseudo-group methods, the following two figures (Figure 12 and Figure 13) and Table 8 are the results.

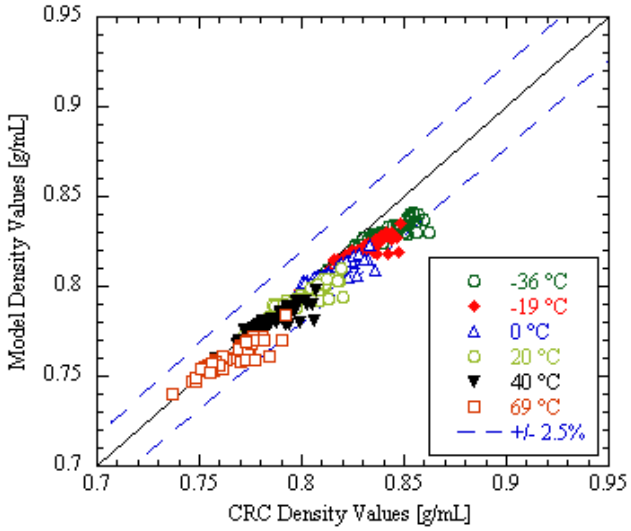

Figure 12. Parity plot with Riazi/Daubert critical property estimates using the optimum fluids, ethane and isopentane.

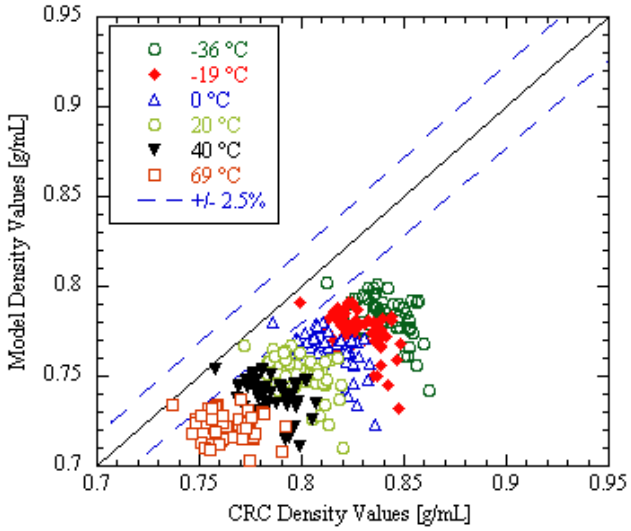

Figure 13. Parity plot with hybrid critical property estimates using the optimum fluids, ethane and isopentane.

Table 8. Comparison of Critical Properties Methods using optimum fluids for the Numerical Regression Method

Method	Reference Fluid #1	Reference Fluid #2	AAD%	Ave%
Numerical Regression	Ethane	Isopentane	0.225	-0.0078
Riazi/Daubert	Ethane	Isopentane	0.59	0.92
Hybrid	Ethane	Isopentane	2.00	6.79

The numerical regression data is also shown in Table 7, and is shown again in Table 8 to facilitate easier comparison. By comparing Figure 10 and Figure 12, as well as comparing Figure 11 and Figure 13, combined with their statistical parameters, it is apparent that reference fluids contribute strongly to the predicted values. For example, when using ethane/isopentane as the reference pairing, the bias is greater than the optimal pairing for both the Riazi/Daubert and Hybrid critical property estimation than with their specific reference fluids. As such, reference fluids selection is an extremely important factor in creating an appropriate predictive model.

4.1.3 Three-Parameter GCSP

A brief examination of three-parameter GCSP was also applied to density with the following triplet of reference fluids; propane, isopentane, and n-pentadecane. These fluids were selected to provide a variety of differing parameters, specifically, a small molecule, an iso-paraffin, and a large molecule, but also be similar to the target fluid (jet fuel). These reference fluids were introduced into the models via equation (20). Results of this study are shown in Table 9 below as well as in Figure 14 to Figure 16.

Table 9. Statistics for 3-Parameter GCSP

Method	AAD%	Ave%
Numerical Regression	0.35	0.62
Riazi/Daubert	0.62	0.84
Hybrid	2.00	7.29

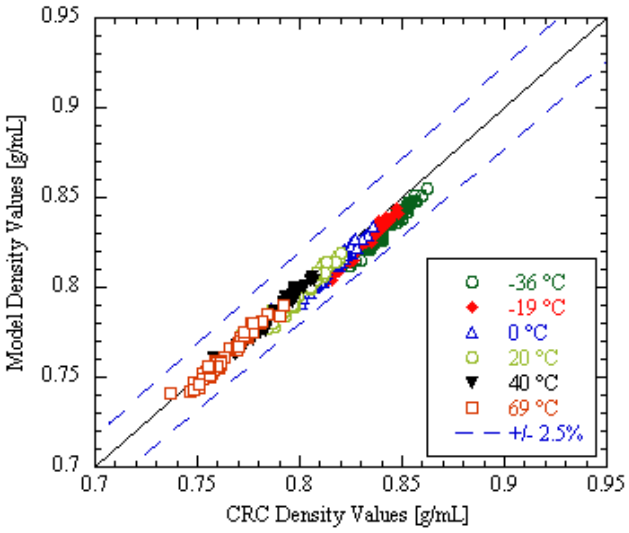

Figure 14. Parity plot of 3-parameter GCSP using numerical regression critical property calculations.

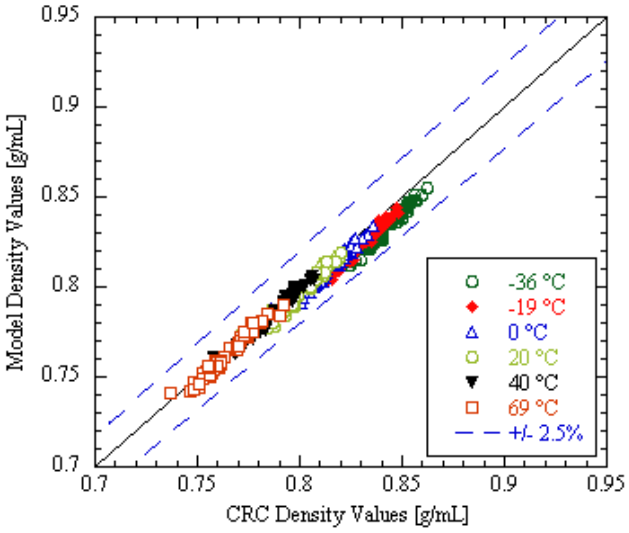

Figure 15. Parity plot 3-parameter GCSP using Riazi/Daubert critical property calculations.

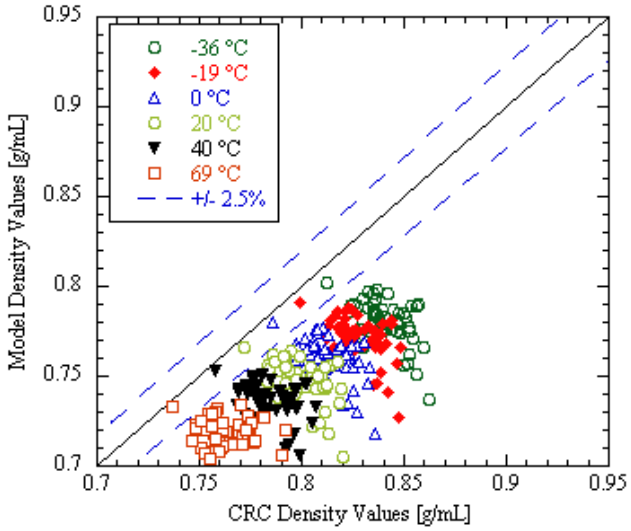

Figure 16. Parity plot of 3-parameter GCSP using hybrid critical property calculations.

The initial results from this study are promising, due to the fact that non-optimized reference fluids were used in this analysis. This fact alone indicates that the three-parameter GCSP could offer improvement over the two-parameter GCSP. For the Riazi/Daubert method in particular there is slight improvement in AAD% (from optimized reference fluids). However, optimization of the reference fluids for the three parameter GCSP case is not straightforward. Due to the complexity of equation (20), it is believed that a non-linear algorithm would be required to determine the optimum reference fluid groups. However, this optimization is outside the scope of this work.

4.2 Viscosity

The utility of GCSP, for a complex mixture, was demonstrated for density, i.e., a thermodynamic property. It is also of interest to apply this method to transport properties, such as viscosity. Equation (10) was used to conduct the study. Similar to the density investigation, the three methods of critical property estimation were applied, as well as

the optimization procedure for reference fluids selection. Figure 17 below shows the log of viscosity of three typical jet fuels plotted against the inverse of temperature. The numerical regression method to determine the pseudo-critical properties, along with the optimized fluid set, was used to generate the figure. As such, the figures present reasonably accurate values for each of the fuels.

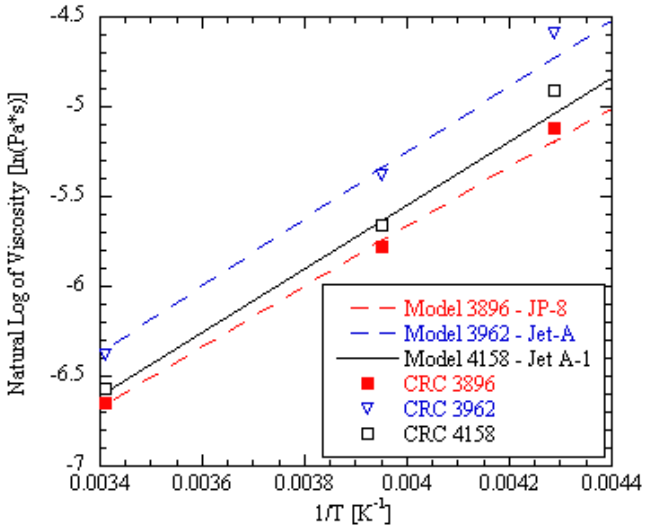

Figure 17. Viscosity profile (in Andrade form) using Method 1 critical properties and optimum reference fluids (n-propylbenzene and n-butylbenzene).

Figure 18 to Figure 20 show the results of the three critical property methods with their optimum reference fluids as a parity plotted against the absolute natural log of viscosity. For each of the three component critical property methods, the optimum reference fluids (Table 10) are different from the optimum reference fluids for density (Table 7) and are, in general, heavier molecular weight fluids. The difference most likely is due to the fact that both trace components and higher molecular weight fluids have a larger effect on density at sub-ambient temperatures due to molecular effects.

Table 10. Optimum Reference Fluids for Viscosity

Method	Reference Fluid #1	Reference Fluid #2	Zone Err%	AAD%	Δ	Ave%
Numerical Regression	n-propylbenzene	n-butylbenzene	0.32	8.44	2.70	1.43
Riazi/Daubert	isooctane	n-Tridecane	0.015	9.50	0.1425	5.36
Hybrid	cumene	n-Tetradecane	-0.0317	9.15	0.29	5.06

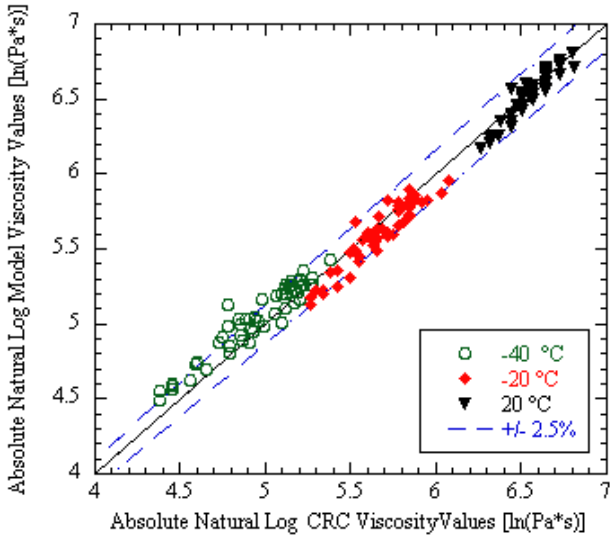

Figure 18. Parity plot of the absolute natural logarithm of viscosity using numerical regression for critical property estimates (Method 1); optimum reference fluids: n-propylbenzene and n-butylbenzene

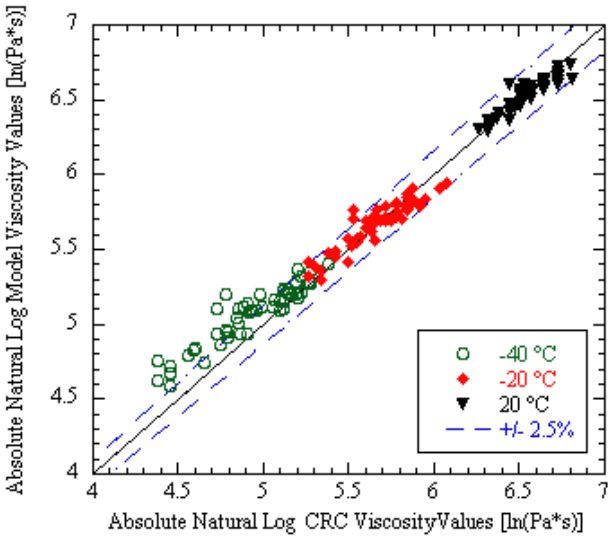

Figure 19. Parity plot of the absolute natural logarithm of viscosity using Riazi/Daubert for critical property estimates (Method 2); optimum reference fluids: isooctane and n-Tridecane

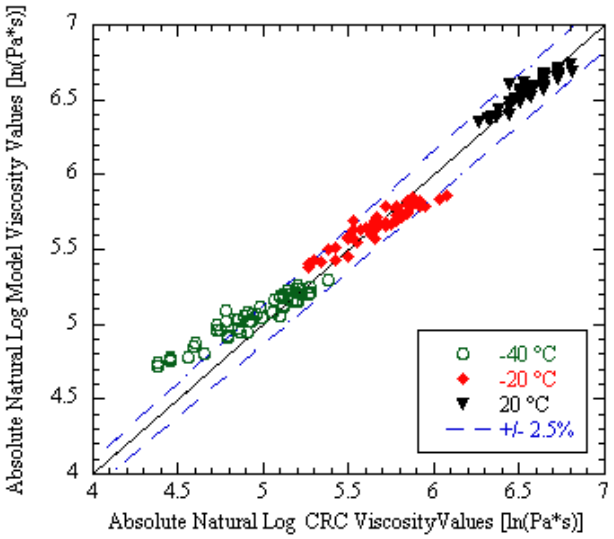

Figure 20. Parity plot of the absolute natural logarithm of viscosity using hybrid method for critical property estimates (Method 3); optimum reference fluids: cumene and n-Tetradecane

It should be noted that at the lowest temperature (-40 °C) the predicted viscosities tend to diverge from the measured values. This could be due to changes in molecular interaction that are unaccounted for within the GCSP model, such as an increase in polarity of some

molecules. Nevertheless, this work provides evidence that GCSP can be applied to a transport property, e.g., viscosity, of a complex fuel mixture. Furthermore, the method is also reasonably accurate at these predictions, provided proper selection of reference fluids and pseudo-critical properties.

CHAPTER 5

CONCLUSIONS AND FUTURE WORK

In summary, information has been presented in this work, but there are some key points which must be highlighted. First and foremost, GCSP can be applied to complex hydrocarbon mixtures, particularly jet fuels, to varying degrees of accuracy. The accuracy is dependent on the component property calculation method as well as the reference fluids that are selected. Furthermore, GCSP can be applied to both thermodynamic and transport properties of these hydrocarbon mixtures. The largest contribution of this work to GCSP, however, is the proof that pseudo-groups can be substituted for pure components within the method and used to predict the desired properties. The last notable aspect of utilizing GCSP is the ability to predict the desired properties as a function of temperature.

A regression-based approach to estimate critical property data for pseudo-groups appeared to provide the most accurate and consistent model predictions (compared to measured values). As such, the recommended method to apply GCSP for jet fuels is to use regression-based pseudo-groups with the optimum reference fluids to predict the density using two-parameter GCSP. This is recommended as it yields the highest overall accuracy of predictions when compared to existing data. For predicting viscosity using

the two-parameter GCSP, the recommended method is to use the numerical regression method with its optimum fluids.

Future investigation(s) should look into other thermodynamic and transport properties. Prime candidates are thermal conductivity, heat capacity, surface tension, and speed of sound, as all of these properties are listed in the specification. Other aspects that could be studied include a more extensive search on reference fluids to see what exact factors are resulting in certain pairings being optimum, an investigation into the optimum three-parameter reference fluid set, and whether a simple mixture could serve as a reference fluid to replace a pure component reference fluid. In order for a simple mixture to be used as a reference fluid, an equation of state would have to be defined, either empirically or through theoretical techniques, such as a Helmholtz energy-based method. By defining this mixture's properties, i.e., density, critical temperature, critical volume, etc., this simple mixture may be able to add complexity to the model via the reference fluids, without increasing the number of parameters of the model. Furthermore, the simple mixture could reflect some of the variety of component families contained within a fuel. One such mixture might be a 50/50 combination of ethane and benzene, which would contribute small molecular information as well as aromatic information into the reference fluid.

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APPENDIX A – Compounds Database

This section contains information obtained from the DIPPR 801 database that was used in the various aspects of this work.

Appendix A.1 DIPPR 801 database compounds

A.1.1 Alkyl-Benzenes (Aromatics)

material or substance name	molecular formula	molecular weight	T_c (K)	V_c (m^3/kmol)	acentric factor, w
benzene	C6H6	78.11	562	0.256	0.210
toluene	C7H8	92.14	592	0.316	0.264
ethylbenzene	C8H10	106.17	617	0.374	0.303
m-xylene	C8H10	106.17	617	0.375	0.326
o-xylene	C8H10	106.17	630	0.37	0.310
p-xylene	C8H10	106.17	616	0.378	0.322
cumene	C9H12	120.19	631	0.434	0.327
5-ethylidene-2-norbornene	C9H12	120.19	629	0.4081	0.314
o-ethyltoluene	C9H12	120.19	650	0.427	0.335
m-ethyltoluene	C9H12	120.19	637	0.427	0.365
p-ethyltoluene	C9H12	120.19	640	0.427	0.367
mesitylene	C9H12	120.19	637	0.433	0.399
n-propylbenzene	C9H12	120.19	638	0.44	0.344
1,2,4-trimethylbenzene	C9H12	120.19	649	0.43	0.379
1,2,3-trimethylbenzene	C9H12	120.19	665	0.414	0.367
vinylnorbornene	C9H12	120.19	626	0.427	0.249
sec-butylbenzene	C10H14	134.22	665	0.497	0.279
tert-butylbenzene	C10H14	134.22	660	0.492	0.267
n-butylbenzene	C10H14	134.22	661	0.497	0.394
p-cymene	C10H14	134.22	652	0.497	0.374
m-cymene	C10H14	134.22	649	0.494	0.378
o-cymene	C10H14	134.22	657	0.49	0.366

o-diethylbenzene	C10H14	134.22	668	0.502	0.340
m-diethylbenzene	C10H14	134.22	663	0.488	0.354
p-diethylbenzene	C10H14	134.22	658	0.497	0.403
2-ethyl-m-xylene	C10H14	134.22	671	0.482	0.407
4-ethyl-m-xylene	C10H14	134.22	665	0.482	0.414
5-ethyl-m-xylene	C10H14	134.22	655	0.482	0.417
2-ethyl-p-xylene	C10H14	134.22	663	0.482	0.411
3-ethyl-o-xylene	C10H14	134.22	680	0.507	0.362
4-ethyl-o-xylene	C10H14	134.22	667	0.49	0.411
isobutylbenzene	C10H14	134.22	650	0.478	0.382
1-methyl-3-n-propylbenzene	C10H14	134.22	654	0.482	0.413
1-methyl-2-n-propylbenzene	C10H14	134.22	662	0.482	0.407
1-methyl-4-n-propylbenzene	C10H14	134.22	656	0.482	0.413
1,2,3,5-tetramethylbenzene	C10H14	134.22	679	0.482	0.424
1,2,4,5-tetramethylbenzene	C10H14	134.22	676	0.482	0.422
1,2,3,4-tetramethylbenzene	C10H14	134.22	693	0.475	0.417
1,2-dimethyl-3-propylbenzene	C11H16	148.24	688	0.586	0.453
1-ethyl-2-isopropylbenzene	C11H16	148.24	666	0.53	0.418
pentamethylbenzene	C11H16	148.24	719	0.538	0.464
n-pentylbenzene	C11H16	148.24	680	0.55	0.438
1,2,4-trimethyl-5-ethylbenzene	C11H16	148.24	687	0.54	0.464
1,2,3-trimethyl-4-ethylbenzene	C11H16	148.24	703	0.531	0.457
1,2,4-trimethyl-3-ethylbenzene	C11H16	148.24	697	0.531	0.457
p-diisopropylbenzene	C12H18	162.27	689	0.598	0.390
m-diisopropylbenzene	C12H18	162.27	684	0.6	0.359
p-tert-butyl ethylbenzene	C12H18	162.27	684	0.605	0.435
hexamethylbenzene	C12H18	162.27	758	0.593	0.496
n-hexylbenzene	C12H18	162.27	698	0.593	0.479
1,3,5-triethylbenzene	C12H18	162.27	678	0.593	0.508
1,2,3-triethylbenzene	C12H18	162.27	683	0.593	0.505
1,2,4-triethylbenzene	C12H18	162.27	684	0.6	0.501
n-heptylbenzene	C13H20	176.30	714	0.648	0.527
1,4-di-tert-butylbenzene	C14H22	190.32	708	0.732	0.502
n-octylbenzene	C14H22	190.32	729	0.703	0.567
1,2,3,5-tetraethylbenzene	C14H22	190.32	708	0.703	0.594
1,3,5-triisopropylbenzene	C15H24	204.35	697	0.739	0.532
n-nonylbenzene	C15H24	204.35	741	0.753	0.633
n-decylbenzene	C16H26	218.38	753	0.813	0.680
pentaethylbenzene	C16H26	218.38	731	0.813	0.670
n-undecylbenzene	C17H28	232.40	764	0.868	0.729
n-dodecylbenzene	C18H30	246.43	780	0.923	0.733
hexaethylbenzene	C18H30	246.43	746	0.923	0.753

1,3,5-tri-tert-butylbenzene	C18H30	246.43	718	0.894	0.487
1,2,4,5-tetraisopropylbenzene	C18H30	246.43	703	0.912706	0.636
n-tridecylbenzene	C19H32	260.46	790	0.978	0.780
n-tetradecylbenzene	C20H34	274.48	800	1.03	0.813
n-pentadecylbenzene	C21H36	288.51	809	1.09	0.857
n-hexadecylbenzene	C22H38	302.54	818	1.14	0.900
n-heptadecylbenzene	C23H40	316.56	826	1.2	0.919
n-octadecylbenzene	C24H42	330.59	834	1.25	0.950

A.1.2 Cyclo-aromatics

material or substance name	molecular formula	molecular weight	T_c (K)	V_c (m^3/kmol)	acentric factor, w
indane	C9H10	118.18	685	0.396	0.309
1,2,3,4-tetrahydronaphthalene	C10H12	132.20	720	0.408	0.335
1-methyltetralin	C11H14	146.23	719	0.497	0.384
1-ethyltetralin	C12H16	160.26	733	0.555	0.429
methylcyclopentadiene dimer	C12H16	160.26	675	0.541	0.423
diamantane	C14H20	188.31	791	0.663	0.163
1-n-hexyl-1,2,3,4-tetrahydronaphthalene	C16H24	216.36	779	0.771	0.589

A.1.3 Di-aromatics

material or substance name	molecular formula	molecular weight	T_c (K)	V_c (m^3/kmol)	acentric factor, w
indene	C9H8	116.16	687	0.368	0.334
naphthalene	C10H8	128.17	748	0.407	0.302
1-methylindene	C10H10	130.19	703	0.436	0.335
2-methylindene	C10H10	130.19	711	0.436	0.351
2-methylnaphthalene	C11H10	142.20	761	0.465	0.378
1-methylnaphthalene	C11H10	142.20	772	0.465	0.342
acenaphthalene	C12H8	152.19	792	0.544	0.399
acenaphthene	C12H10	154.21	803	0.553	0.381
biphenyl	C12H10	154.21	773	0.497	0.403
2,7-dimethylnaphthalene	C12H12	156.22	775	0.6	0.448

2,6-dimethylnaphthalene	C12H12	156.22	777	0.52	0.418
1-ethylnaphthalene	C12H12	156.22	776	0.52	0.407
2-ethylnaphthalene	C12H12	156.22	771	0.52	0.421
1,2,3-trimethylindene	C12H14	158.24	726	0.529	0.442
fluorene	C13H10	166.22	826	0.524	0.404
diphenylmethane	C13H12	168.23	760	0.563	0.482
1-n-propylnaphthalene	C13H14	170.25	782	0.575	0.455
cis-stilbene	C14H12	180.25	784	0.596	0.476
trans-stilbene	C14H12	180.25	820	0.607	0.487
1,2-diphenylethane	C14H14	182.26	780	0.616	0.488
1,1-diphenylethane	C14H14	182.26	775	0.604	0.457
1-n-butylnaphthalene	C14H16	184.28	792	0.631	0.495
2,6-diethylnaphthalene	C14H16	184.28	807	0.63	0.512
2,2-diphenyl propane	C15H16	196.29	780	0.6409	0.461
1-n-pentylnaphthalene	C15H18	198.30	803	0.686	0.535
1-(4-ethylphenyl)-2-phenylethane	C16H18	210.31	771	0.704	0.578
1-n-hexylnaphthalene	C16H20	212.33	813	0.741	0.587
2,4-diphenyl-4-methylpentene-1	C18H20	236.35	835	0.839	0.547
2,3-dimethyl-2,3-diphenylbutane	C18H22	238.37	805	0.781	0.521
1-(4-ethylphenyl)-2-(4-ethylphenyl)ethane	C18H22	238.37	781	0.799	0.586
1-n-nonylnaphthalene	C19H26	254.41	835	0.906	0.722
1-n-decylnaphthalene	C20H28	268.44	844	0.961	0.746

A.1.4 Di-cycloparaffins

material or substance name	molecular formula	molecular weight	T_c (K)	V_c (m^3/kmol)	acentric factor, w
bicyclo[2.2.1]heptane	C7H12	96.17	594	0.352	0.164
bicyclo[2.2.2]octane	C8H14	110.20	625	0.405	0.205
camphene	C10H16	136.23	638	0.499	0.296
cis-decahydronaphthalene	C10H18	138.25	704	0.48	0.279
trans-decahydronaphthalene	C10H18	138.25	687	0.48	0.299
bicyclohexyl	C12H22	166.30	727	0.598	0.428

A.1.5 Iso-paraffins

material or substance name	molecular formula	molecular weight	T_c (K)	V_c (m^3/kmol)	acentric factor, w
isobutane	C4H10	58.12	408	0.259	0.184
isopentane	C5H12	72.15	460	0.306	0.228
neopentane	C5H12	72.15	434	0.307	0.196
2,2-dimethylbutane	C6H14	86.18	489	0.358	0.234
2,3-dimethylbutane	C6H14	86.18	500	0.361	0.249
3-methylpentane	C6H14	86.18	505	0.368	0.270
2-methylpentane	C6H14	86.18	498	0.368	0.279
2,4-dimethylpentane	C7H16	100.20	520	0.418	0.302
2,3-dimethylpentane	C7H16	100.20	537	0.393	0.296
3,3-dimethylpentane	C7H16	100.20	536	0.414	0.268
2,2-dimethylpentane	C7H16	100.20	521	0.416	0.287
3-ethylpentane	C7H16	100.20	541	0.416	0.309
2-methylhexane	C7H16	100.20	530	0.421	0.328
3-methylhexane	C7H16	100.20	535	0.404	0.320
2,2,3-trimethylbutane	C7H16	100.20	531	0.398	0.250
2,5-dimethylhexane	C8H18	114.23	550	0.482	0.358
3,3-dimethylhexane	C8H18	114.23	562	0.443	0.320
2,2-dimethylhexane	C8H18	114.23	550	0.478	0.338
2,4-dimethylhexane	C8H18	114.23	554	0.472	0.344
3,4-dimethylhexane	C8H18	114.23	569	0.466	0.338
2,3-dimethylhexane	C8H18	114.23	564	0.468	0.346
3-ethylhexane	C8H18	114.23	566	0.455	0.361
2-methyl-3-ethylpentane	C8H18	114.23	567	0.442	0.330
3-methyl-3-ethylpentane	C8H18	114.23	577	0.455	0.305
3-methylheptane	C8H18	114.23	564	0.464	0.372
2-methylheptane	C8H18	114.23	560	0.488	0.380
4-methylheptane	C8H18	114.23	562	0.476	0.371
2,2,3,3-tetramethylbutane	C8H18	114.23	568	0.461	0.245
2,3,3-trimethylpentane	C8H18	114.23	574	0.455	0.290
2,2,3-trimethylpentane	C8H18	114.23	564	0.436	0.297
2,3,4-trimethylpentane	C8H18	114.23	566	0.46	0.315
2,2,4-trimethylpentane	C8H18	114.23	544	0.468	0.303
3,3-diethylpentane	C9H20	128.26	610	0.473	0.338
2,4-dimethyl-3-ethylpentane	C9H20	128.26	591	0.512	0.353
2,2-dimethyl-3-ethylpentane	C9H20	128.26	590	0.511	0.335
2,2-dimethylheptane	C9H20	128.26	577	0.519	0.391

2,6-dimethylheptane	C9H20	128.26	579	0.52	0.393
3-ethylheptane	C9H20	128.26	590	0.528	0.408
2-methyloctane	C9H20	128.26	583	0.541	0.460
4-methyloctane	C9H20	128.26	588	0.523	0.413
3-methyloctane	C9H20	128.26	590	0.529	0.412
2,2,4,4-tetramethylpentane	C9H20	128.26	575	0.504	0.314
2,3,3,4-tetramethylpentane	C9H20	128.26	608	0.493	0.314
2,2,3,3-tetramethylpentane	C9H20	128.26	608	0.478	0.305
2,2,3,4-tetramethylpentane	C9H20	128.26	593	0.49	0.314
2,4,4-trimethylhexane	C9H20	128.26	581	0.511	0.352
2,2,5-trimethylhexane	C9H20	128.26	570	0.519	0.345
2,6-dimethyloctane	C10H22	142.28	606	0.575	0.439
2,2-dimethyloctane	C10H22	142.28	602	0.574	0.429
2,7-dimethyloctane	C10H22	142.28	604	0.575	0.442
2,5-dimethyloctane	C10H22	142.28	603	0.575	0.440
2,4-dimethyloctane	C10H22	142.28	600	0.575	0.434
4-methylnonane	C10H22	142.28	610	0.583	0.465
2-methylnonane	C10H22	142.28	610	0.583	0.472
5-methylnonane	C10H22	142.28	610	0.583	0.456
3-methylnonane	C10H22	142.28	613	0.583	0.465
2,2,5,5-tetramethylhexane	C10H22	142.28	581	0.584	0.377
2,2,3,3-tetramethylhexane	C10H22	142.28	623	0.557	0.366
3,3,5-trimethylheptane	C10H22	142.28	610	0.577	0.385
2,3-dimethyloctane	C10H22	142.28	613	0.599	0.425
3-methylundecane	C12H26	170.33	655	0.693	0.552
2,2,4,4,6,8,8-heptamethylnonane	C16H34	226.44	692	0.863	0.548
squalane	C30H62	422.81	863	1.64	0.915

A.1.6 Monocyclo-paraffins

material or substance name	molecular formula	molecular weight	T_c (K)	V_c (m^3/kmol)	acentric factor, w
cyclopropane	C3H6	42.08	398	0.162	0.128
cyclobutane	C4H8	56.11	460	0.21	0.185
cyclopentane	C5H10	70.13	512	0.26	0.195
cyclohexane	C6H12	84.16	554	0.308	0.208
methylcyclopentane	C6H12	84.16	533	0.319	0.229
cycloheptane	C7H14	98.19	604	0.353	0.241
trans-1,3-dimethylcyclopentane	C7H14	98.19	553	0.36	0.270

cis-1,3-dimethylcyclopentane	C7H14	98.19	551	0.36	0.274
trans-1,2-dimethylcyclopentane	C7H14	98.19	553	0.36	0.270
cis-1,2-dimethylcyclopentane	C7H14	98.19	565	0.37	0.266
1,1-dimethylcyclopentane	C7H14	98.19	547	0.36	0.272
ethylcyclopentane	C7H14	98.19	570	0.375	0.270
methylcyclohexane	C7H14	98.19	572	0.369	0.236
cyclooctane	C8H16	112.21	647	0.41	0.252
cis-1,4-dimethylcyclohexane	C8H16	112.21	598	0.46	0.231
trans-1,3-dimethylcyclohexane	C8H16	112.21	598	0.46	0.233
cis-1,3-dimethylcyclohexane	C8H16	112.21	591	0.45	0.237
trans-1,2-dimethylcyclohexane	C8H16	112.21	596	0.46	0.238
cis-1,2-dimethylcyclohexane	C8H16	112.21	606	0.46	0.232
1,1-dimethylcyclohexane	C8H16	112.21	591	0.45	0.233
trans-1,4-dimethylcyclohexane	C8H16	112.21	588	0.45	0.255
ethylcyclohexane	C8H16	112.21	609	0.43	0.246
isopropylcyclopentane	C8H16	112.21	593	0.42	0.303
1-methyl-1-ethylcyclopentane	C8H16	112.21	582	0.428	0.330
n-propylcyclopentane	C8H16	112.21	596	0.428	0.327
1-cis-2-trans-4-trimethylcyclopentane	C8H16	112.21	579	0.417	0.278
1-cis-2-trans-3-trimethylcyclopentane	C8H16	112.21	580	0.417	0.280
1,1,3-trimethylcyclopentane	C8H16	112.21	570	0.417	0.212
1,1,2-trimethylcyclopentane	C8H16	112.21	580	0.417	0.252
n-butylcyclopentane	C9H18	126.24	621	0.483	0.372
isopropylcyclohexane	C9H18	126.24	627	0.464	0.330
n-propylcyclohexane	C9H18	126.24	639	0.477	0.260
1-trans-3,5-trimethylcyclohexane	C9H18	126.24	602	0.472	0.367
n-butylcyclohexane	C10H20	140.27	667	0.534	0.274
1,1-diethylcyclohexane	C10H20	140.27	643	0.534	0.404
trans-1,4-diethylcyclohexane	C10H20	140.27	650	0.527	0.385

1,2,3,4-tetramethylcyclohexane	C10H20	140.27	642	0.528	0.402
iso-butylcyclohexane	C10H20	140.27	642	0.519	0.354
tert-butylcyclohexane	C10H20	140.27	652	0.51	0.299
sec-butylcyclohexane	C10H20	140.27	654	0.515	0.352
n-decylcyclohexane	C16H32	224.43	751	0.858	0.663

A.1.7 n-paraffins

material or substance name	molecular formula	molecular weight	T_c (K)	V_c (m^3/kmol)	acentric factor, w
n-heptane	C7H16	100.20	540	0.428	0.349
n-octane	C8H18	114.23	569	0.486	0.400
n-nonane	C9H20	128.26	595	0.551	0.443
n-decane	C10H22	142.28	618	0.617	0.492
n-undecane	C11H24	156.31	639	0.685	0.530
n-dodecane	C12H26	170.33	658	0.755	0.576
n-tridecane	C13H28	184.36	675	0.826	0.617
n-tetradecane	C14H30	198.39	693	0.897	0.643
n-pentadecane	C15H32	212.41	708	0.969	0.686
n-hexadecane	C16H34	226.44	723	1.04	0.717
n-heptadecane	C17H36	240.47	736	1.11	0.770
n-octadecane	C18H38	254.49	747	1.19	0.811
n-nonadecane	C19H40	268.52	758	1.26	0.852
n-eicosane	C20H42	282.55	768	1.34	0.907
n-heneicosane	C21H44	296.57	778	1.41	0.942
n-docosane	C22H46	310.60	787	1.48	0.972
n-tricosane	C23H48	324.63	796	1.56	1.026

A.1.8 Tricyclo-paraffins

material or substance name	molecular formula	molecular weight	T_c (K)	V_c (m^3/kmol)	acentric factor, w
2-norbornene	C7H10	94.15	583	0.337	0.159
methylnorbornene	C8H12	108.18	600	0.377	0.211
ethylnorbornene	C9H14	122.21	625	0.437	0.261
adamantane	C10H16	136.23	703	0.485	0.185
1,3-dimethyladamantane	C12H20	164.29	708	0.57	0.293

Appendix A.2 Reference Fluid Property Correlations

A.2.1 Density Reference Fluids

Name	MW	T_c	V_c	ω	A	B	C	D
methane	16.04246	190.564	0.0986	0.011548	2.9214	0.28976	190.56	0.28881
ethane	30.06904	305.32	0.1455	0.099493	1.9122	0.27937	305.32	0.29187
propane	44.09562	369.83	0.2	0.152291	1.3757	0.27453	369.83	0.29359
n-butane	58.1222	425.12	0.255	0.200164	1.0677	0.27188	425.12	0.28688
isobutane	58.1222	407.8	0.259	0.183521	1.0631	0.27506	407.8	0.2758
cyclopentane	70.1329	511.7	0.26	0.194874	1.0897	0.28356	511.7	0.25142
isopentane	72.14878	460.4	0.306	0.227875	0.91991	0.27815	460.4	0.28667
benzene	78.11184	562.05	0.256	0.2103	1.0259	0.26666	562.05	0.28394
cyclohexane	84.15948	553.8	0.308	0.208054	0.88998	0.27376	553.8	0.28571
toluene	92.13842	591.75	0.316	0.264012	0.8792	0.27136	591.75	0.29241
ethylcyclopentane	98.18606	569.5	0.375	0.270095	0.71751	0.26903	569.5	0.27733
methylcyclohexane	98.18606	572.1	0.369	0.236055	0.73109	0.26971	572.1	0.29185
ethylbenzene	106.165	617.15	0.374	0.30347	0.70041	0.26162	617.15	0.28454
1,1-dimethyl-cyclohexane	112.2126	591.15	0.45	0.232569	0.55873	0.25143	591.15	0.27758
ethylcyclohexane	112.2126	609.15	0.43	0.245525	0.61587	0.26477	609.15	0.28054
2,2,4-trimethylpentane	114.2285	543.8	0.468	0.303455	0.59059	0.27424	543.8	0.2847
n-octane	114.2285	568.7	0.486	0.399552	0.5266	0.25693	568.7	0.28571
cumene	120.1916	631	0.434	0.327406	0.58711	0.25583	631	0.28494
n-propylbenzene	120.1916	638.35	0.44	0.344391	0.57233	0.25171	638.35	0.29616
naphthalene	128.1705	748.4	0.407	0.302034	0.6348	0.25838	748.4	0.27727
n-nonane	128.2551	594.6	0.551	0.44346	0.46321	0.25444	594.6	0.28571
1,2,3,4-tetrahydro-naphthalene	132.2023	720	0.408	0.335255	0.67717	0.27772	720	0.2878
n-butylbenzene	134.2182	660.5	0.497	0.394149	0.50812	0.25238	660.5	0.29373
n-decane	142.2817	617.7	0.617	0.492328	0.41084	0.25175	617.7	0.28571

Equation: $\rho = \frac{A}{B^{\left[1+\left(1-\frac{T}{C}\right)^{D}\right]}}$

Information in this table comes from the DIPPR 801 database.

A.2.2 Viscosity Reference Fluids

Name	MW	T_c	V_c	ω	A	B	C	D	E
methane	16.04246	190.564	0.0986	0.011548	-6.1572	178.15	-0.95239	-9.1E-24	10
ethane	30.06904	305.32	0.1455	0.099493	-7.0046	276.38	-0.6087	-3.1E-18	7
propane	44.09562	369.83	0.2	0.152291	-17.156	646.25	1.1101	-7.3E-11	4
n-butane	58.1222	425.12	0.255	0.200164	-7.2471	534.82	-0.57469	-4.7E-27	10
n-pentane	72.14878	469.7	0.313	0.251506	-53.509	1836.6	7.1409	-2E-05	2
benzene	78.11184	562.05	0.256	0.2103	7.5117	294.68	-2.794	0	0
n-hexane	86.17536	507.6	0.371	0.301261	-56.569	2140.5	7.5175	-1.8E-05	2
toluene	92.13842	591.75	0.316	0.264012	-226.08	6805.7	37.542	-0.06085	1
n-heptane	100.2019	540.2	0.428	0.349469	-98.159	3592.6	14.197	-3E-05	2
ethylbenzene	106.165	617.15	0.374	0.30347	-13.563	1208.6	0.377	0	0
cyclooctane	112.2126	647.2	0.41	0.252353	-10.716	1140.5	-0.04774	0	0
1,1-dimethyl-cyclohexane	112.2126	591.15	0.45	0.232569	-22.11	1673	1.641	0	0
ethylcyclohexane	112.2126	609.15	0.43	0.245525	-23.305	1617.8	1.8473	0	0
2,2,4-trimethyl-pentane	114.2285	543.8	0.468	0.303455	-11.432	1074	0.015358	0	0
n-octane	114.2285	568.7	0.486	0.399552	-98.805	3905.5	14.103	-2.5E-05	2
cumene	120.1916	631	0.434	0.327406	-11.756	1483.1	-0.04039	0	0
n-propylbenzene	120.1916	638.35	0.44	0.344391	-18.282	1549.7	1.0454	0	0
naphthalene	128.1705	748.4	0.407	0.302034	-19.308	1822.5	1.218	0	0
n-nonane	128.2551	594.6	0.551	0.44346	-68.54	3165.3	9.0919	-1.4E-05	2
1,2,3,4-tetrahydro-naphthalene	132.2023	720	0.408	0.335255	-118.86	5829.5	16.605	-1.7E-05	2
n-butylbenzene	134.2182	660.5	0.497	0.394149	-11.273	1528.8	-0.10761	0	0
n-decane	142.2817	617.7	0.617	0.492328	-12.875	1745.1	0	0	0
pentamethyl-benzene	148.2447	719.15	0.538	0.46366	-12.784	1937.1	0	0	0
biphenyl	154.2078	773	0.497	0.402873	-9.9265	1576.3	-0.21119	0	0
n-hexylbenzene	162.2713	698	0.593	0.478964	-11.467	1529	0	0	0
n-dodecane	170.3348	658	0.755	0.576385	-11.513	1368.4	0.000159	0	0
n-tridecane	184.3614	675	0.826	0.617397	-111.98	5468.6	15.579	-1.7E-05	2
n-octylbenzene	190.3245	729	0.703	0.567041	-13.19	1818.7	0.22498	0	0
n-tetradecane	198.388	693	0.897	0.643017	-136.73	6421.3	19.493	-2.3E-05	2
n-nonylbenzene	204.3511	741	0.753	0.633063	-69.526	4600.4	8.4663	0	0
1-n-hexyl-naphthalene	212.33	813	0.741	0.587382	-10.976	1633.1	0	0	0
n-pentadecane	212.4146	708	0.969	0.68632	-19.299	2088.6	1.1091	0	0
1-n-hexyl-1,2,3,4-tetrahydro-naphthalene	216.3618	779	0.771	0.588792	-4.971	1345.1	-0.92207	0	0

Equation: $\eta = e^{\left[A + \frac{B}{T} + C * \ln T + D * T^{E}\right]}$

Information in the above table comes from the DIPPR 801 Database.

APPENDIX B – Pseudo-Groups/Reference Fluids

This appendix contains data from the pseudo-group methods. This is followed by the reference fluids optimization results.

Appendix B.1 – Pseudo-Groups

B.1.1 Numerical Regression

Tabulated critical property data used for pseudo-groups. Database component identifies the method used to determine T_c, V_c, and ω.

Name	molecular formula	MW	Tc (K)	Vc (m3/kmol)	ω	Database Component
C00-benzene	C6H6	78.112	562.05	0.2560	0.2103	DIPPR
C01-benzene	C7H8	92.138	591.75	0.3160	0.264	DIPPR
C02-benzene	C8H10	106.166	570.79	0.3763	0.3068	REGRESSION
C03-benzene	C9H12	120.193	598.30	0.4308	0.3474	REGRESSION
C04-benzene	C10H14	134.22	622.13	0.4853	0.388	REGRESSION
C05-benzene	C11H16	148.247	643.14	0.5398	0.4286	REGRESSION
C06-benzene	C12H18	162.274	661.94	0.5943	0.4692	REGRESSION
C07-benzene	C13H20	176.301	678.95	0.6488	0.5098	REGRESSION
C08-benzene	C14H22	190.328	694.48	0.7033	0.5504	REGRESSION
C09-benzene	C15H24	204.355	708.76	0.7578	0.591	REGRESSION
C10+ benzene	C16H26	218.382	721.98	0.8123	0.6316	REGRESSION
cycloaromatic-C09	C9H10	118.176	684.90	0.3960	0.3092	DIPPR

cycloaromatic-C10	C10H12	132.202	720.00	0.4080	0.3353	DIPPR
cycloaromatic-C11	C11H14	146.229	719.30	0.4970	0.3836	DIPPR
cycloaromatic-C12	C12H16	160.255	733.00	0.5550	0.4292	DIPPR
cycloaromatic-C13	C13H18	174.283	762.00	0.6090	0.466	REGRESSION
cycloaromatic-C14	C14H20	188.309	791.00	0.6630	0.5068	REGRESSION
cycloaromatic-C15+	C16H24	216.362	779.00	0.7710	0.5888	DIPPR
diaromatic-C10	C10H8	128.171	748.40	0.4070	0.302	DIPPR
diaromatic-C11	C11H10	142.195	751.97	0.4713	0.3756	REGRESSION
diaromatic-C12	C12H12	156.222	765.06	0.5216	0.4103	REGRESSION
diaromatic-C13	C13H14	170.249	777.11	0.5719	0.445	REGRESSION
diaromatic-C14+	C14H16	184.276	788.26	0.6222	0.4797	REGRESSION
dicyclo-C08	C8H14	110.199	629.95	0.3968	0.2032	REGRESSION
dicyclo-C09	C9H16	124.226	660.59	0.4441	0.2544	REGRESSION
dicyclo-C10	C10H18	138.253	688.00	0.4914	0.3056	REGRESSION
dicyclo-C11	C11H20	152.28	712.80	0.5387	0.3568	REGRESSION
dicyclo-C12	C12H22	166.307	735.43	0.5860	0.408	REGRESSION
dicyclo-C13	C13H24	180.334	756.26	0.6333	0.4592	REGRESSION
dicyclo-C14	C14H26	194.361	775.54	0.6806	0.5104	REGRESSION
dicyclo-C15	C15H28	208.388	793.49	0.7279	0.5616	REGRESSION
dicyclo-C16	C16H30	222.415	810.28	0.7752	0.6128	REGRESSION
dicyclo-C17+	C17H32	236.442	826.05	0.8225	0.664	REGRESSION
iso-C07-	C7H16	100.202	530.93	0.4118	0.3074	REGRESSION
iso-C08	C8H18	114.229	560.40	0.4651	0.3371	REGRESSION
iso-C09	C9H20	128.255	586.46	0.5184	0.3668	REGRESSION
iso-C10	C10H22	142.282	609.81	0.5717	0.3965	REGRESSION
iso-C11	C11H24	156.308	630.96	0.6250	0.4262	REGRESSION
iso-C12	C12H26	170.335	650.30	0.6783	0.4559	REGRESSION
iso-C13	C13H28	184.361	668.10	0.7316	0.4856	REGRESSION
iso-C14	C14H30	198.388	684.60	0.7849	0.5153	REGRESSION
iso-C15	C15H32	212.415	699.96	0.8382	0.545	REGRESSION
iso-C16	C16H34	226.441	714.35	0.8915	0.5747	REGRESSION
iso-C17	C17H36	240.468	727.87	0.9448	0.6044	REGRESSION
iso-C18	C18H38	254.494	740.63	0.9981	0.6341	REGRESSION
iso-C19	C19H40	268.521	752.70	1.0514	0.6638	REGRESSION
iso-C20	C20H42	282.547	764.15	1.1047	0.6935	REGRESSION
iso-C21	C21H44	296.574	775.05	1.1580	0.7232	REGRESSION
iso-C22	C22H46	310.601	785.45	1.2113	0.7529	REGRESSION
iso-C23	C23H48	324.627	795.39	1.2646	0.7826	REGRESSION
iso-C24	C24H50	338.654	804.90	1.3179	0.8123	REGRESSION
monocyclo-C07-	C7H14	98.189	569.31	0.3723	0.2443	REGRESSION

monocyclo-C08	C8H16	112.216	597.26	0.4257	0.2817	REGRESSION
monocyclo-C09	C9H18	126.243	621.92	0.4791	0.3191	REGRESSION
monocyclo-C10	C10H20	140.27	643.98	0.5325	0.3565	REGRESSION
monocyclo-C11	C11H22	154.297	663.94	0.5859	0.3939	REGRESSION
monocyclo-C12	C12H24	168.324	682.16	0.6393	0.4313	REGRESSION
monocyclo-C13	C13H26	182.351	698.91	0.6927	0.4687	REGRESSION
monocyclo-C14	C14H28	196.378	714.43	0.7461	0.5061	REGRESSION
monocyclo-C15	C15H30	210.405	728.87	0.7995	0.5435	REGRESSION
monocyclo-C16	C16H32	224.432	742.39	0.8529	0.5809	REGRESSION
monocyclo-C17	C17H34	238.459	755.08	0.9063	0.6183	REGRESSION
monocyclo-C18	C18H36	252.486	767.05	0.9597	0.6557	REGRESSION
monocyclo-C19+	C19H38	266.513	778.37	1.0131	0.6931	REGRESSION
n-C07	C7H16	100.202	540.20	0.4280	0.3495	DIPPR
n-C08	C8H18	114.229	568.70	0.4860	0.3996	DIPPR
n-C09	C9H20	128.255	594.60	0.5510	0.4435	DIPPR
n-C10	C10H22	142.282	617.70	0.6170	0.4923	DIPPR
n-C11	C11H24	156.308	639.00	0.6850	0.5303	DIPPR
n-C12	C12H26	170.335	658.00	0.7550	0.5764	DIPPR
n-C13	C13H28	184.361	675.00	0.8260	0.6174	DIPPR
n-C14	C14H30	198.388	693.00	0.8970	0.643	DIPPR
n-C15	C15H32	212.415	708.00	0.9690	0.6863	DIPPR
n-C16	C16H34	226.441	723.00	1.0400	0.7174	DIPPR
n-C17	C17H36	240.468	736.00	1.1100	0.7697	DIPPR
n-C18	C18H38	254.494	747.00	1.1900	0.8114	DIPPR
n-C19	C19H40	268.521	758.00	1.2600	0.8522	DIPPR
n-C20	C20H42	282.547	768.00	1.3400	0.9069	DIPPR
n-C21	C21H44	296.574	778.00	1.4100	0.942	DIPPR
n-C22	C22H46	310.601	787.00	1.4800	0.9722	DIPPR
n-C23	C23H48	324.627	796.00	1.5600	1.0262	DIPPR
tricyclo-C10	C10H16	136.234	703.00	0.4850	0.1853	REGRESSION
tricyclo-C11	C11H18	150.263	705.50	0.5275	0.2394	REGRESSION
tricyclo-C12	C12H20	164.287	708.00	0.5700	0.2935	REGRESSION

B.1.2 Riazi Estimation

In this table, the critical pressure and boiling point estimations are included as they were used to calculate the acentric factor.

Name	molecular formula	MW	Tc (K)	Vc (m3/kmol)	P_c (Bar)	T_b	ω_{L-K}
C00-benzene	C6H6	78.114	543.91	0.2670	43.4	352.87	0.2794
C01-benzene	C7H8	92.141	592.45	0.3173	40.6	385.25	0.2664
C02-benzene	C8H10	106.168	623.82	0.3728	36.7	412.96	0.2991
C03-benzene	C9H12	120.195	647.33	0.4312	32.9	437.96	0.3485
C04-benzene	C10H14	134.222	666.62	0.4912	29.6	461.08	0.4056
C05-benzene	C11H16	148.249	683.35	0.5525	26.7	482.78	0.4673
C06-benzene	C12H18	162.276	698.36	0.6146	24.2	503.32	0.5320
C07-benzene	C13H20	176.303	712.10	0.6775	22.0	522.89	0.5991
C08-benzene	C14H22	190.330	724.86	0.7408	20.2	541.61	0.6683
C09-benzene	C15H24	204.357	736.81	0.8047	18.5	559.60	0.7396
C10+ benzene	C16H26	218.384	748.08	0.8689	17.1	576.93	0.8131
cycloaromatic-C09	C9H10	118.179	616.58	0.4356	32.2	437.02	0.5714
cycloaromatic-C10	C10H12	132.206	646.28	0.4918	29.8	462.05	0.5855
cycloaromatic-C11	C11H14	146.233	668.98	0.5511	27.3	484.86	0.6265
cycloaromatic-C12	C12H16	160.260	687.53	0.6123	25.0	506.08	0.6822
cycloaromatic-C13	C13H18	174.287	703.40	0.6749	22.9	526.08	0.7473
cycloaromatic-C14	C14H20	188.314	717.44	0.7385	21.0	545.09	0.8192
cycloaromatic-C15+	C16H24	202.341	730.13	0.8029	19.3	563.26	0.8967
diaromatic-C10	C10H8	128.174	485.15	0.6007	21.8	441.66	5.3852
diaromatic-C11	C11H10	142.201	554.34	0.6241	23.3	474.61	2.7363
diaromatic-C12	C12H12	156.228	601.88	0.6662	23.2	501.68	2.0989
diaromatic-C13	C13H14	170.255	636.52	0.7177	22.3	525.29	1.8721
diaromatic-C14+	C14H16	184.282	663.09	0.7747	21.1	546.65	1.7999
dicyclo-C08	C8H14	110.200	616.06	0.4060	32.6	405.44	0.2357
dicyclo-C09	C9H16	124.227	635.95	0.4653	28.9	429.41	0.2913
dicyclo-C10	C10H18	138.254	654.43	0.5250	25.9	452.03	0.3456
dicyclo-C11	C11H20	152.281	671.68	0.5851	23.5	473.51	0.3989
dicyclo-C12	C12H22	166.308	687.85	0.6455	21.4	493.97	0.4516
dicyclo-C13	C13H24	180.335	703.08	0.7062	19.6	513.55	0.5039
dicyclo-C14	C14H26	194.362	717.46	0.7672	18.0	532.33	0.5560
dicyclo-C15	C15H28	208.389	731.07	0.8283	16.6	550.41	0.6082
dicyclo-C16	C16H30	222.416	743.99	0.8897	15.4	567.83	0.6607
dicyclo-C17+	C17H32	236.443	756.27	0.9512	14.3	584.67	0.7136

iso-C07-	C7H16	100.205	533.05	0.4136	28.5	365.94	0.3561
iso-C08	C8H18	114.232	562.77	0.4695	25.8	392.24	0.3843
iso-C09	C9H20	128.259	589.51	0.5258	23.4	416.83	0.4136
iso-C10	C10H22	142.286	613.83	0.5825	21.4	439.99	0.4435
iso-C11	C11H24	156.313	636.15	0.6394	19.7	461.93	0.4737
iso-C12	C12H26	170.340	656.77	0.6965	18.2	482.80	0.5042
iso-C13	C13H28	184.367	675.95	0.7539	16.8	502.73	0.5348
iso-C14	C14H30	198.394	693.86	0.8114	15.6	521.83	0.5656
iso-C15	C15H32	212.421	710.67	0.8691	14.6	540.19	0.5966
iso-C16	C16H34	226.448	726.49	0.9270	13.6	557.87	0.6278
iso-C17	C17H36	240.475	741.43	0.9850	12.7	574.94	0.6592
iso-C18	C18H38	254.502	755.57	1.0432	11.9	591.45	0.6908
iso-C19	C19H40	268.529	768.99	1.1014	11.2	607.44	0.7227
iso-C20	C20H42	282.556	781.75	1.1597	10.5	622.95	0.7550
iso-C21	C21H44	296.583	793.91	1.2181	9.9	638.02	0.7876
iso-C22	C22H46	310.610	805.51	1.2766	9.4	652.67	0.8208
iso-C23	C23H48	324.637	816.59	1.3351	8.8	666.94	0.8544
iso-C24	C24H50	338.664	827.20	1.3938	8.3	680.84	0.8887
monocyclo-C07-	C7H14	98.189	565.97	0.3777	32.8	373.14	0.2447
monocyclo-C08	C8H16	112.216	591.40	0.4353	29.1	399.03	0.2911
monocyclo-C09	C9H18	126.243	614.54	0.4933	26.2	423.27	0.3362
monocyclo-C10	C10H20	140.270	635.81	0.5516	23.7	446.14	0.3801
monocyclo-C11	C11H22	154.297	655.48	0.6102	21.6	467.82	0.4233
monocyclo-C12	C12H24	168.324	673.78	0.6691	19.8	488.47	0.4659
monocyclo-C13	C13H26	182.351	690.90	0.7282	18.2	508.21	0.5081
monocyclo-C14	C14H28	196.378	706.97	0.7876	16.8	527.15	0.5501
monocyclo-C15	C15H30	210.405	722.11	0.8471	15.6	545.35	0.5919
monocyclo-C16	C16H32	224.432	736.42	0.9067	14.5	562.90	0.6338
monocyclo-C17	C17H34	238.459	749.97	0.9665	13.5	579.85	0.6759
monocyclo-C18	C18H36	252.486	762.84	1.0264	12.6	596.24	0.7183
monocyclo-C19+	C19H38	266.513	775.09	1.0865	11.8	612.13	0.7611
n-C07	C7H16	100.205	533.05	0.4136	28.5	365.94	0.3561
n-C08	C8H18	114.232	562.77	0.4695	25.8	392.24	0.3843
n-C09	C9H20	128.259	589.51	0.5258	23.4	416.83	0.4136
n-C10	C10H22	142.286	613.83	0.5825	21.4	439.99	0.4435
n-C11	C11H24	156.313	636.15	0.6394	19.7	461.93	0.4737
n-C12	C12H26	170.340	656.77	0.6965	18.2	482.80	0.5042
n-C13	C13H28	184.367	675.95	0.7539	16.8	502.73	0.5348
n-C14	C14H30	198.394	693.86	0.8114	15.6	521.83	0.5656
n-C15	C15H32	212.421	710.67	0.8691	14.6	540.19	0.5966
n-C16	C16H34	226.448	726.49	0.9270	13.6	557.87	0.6278

n-C17	C17H36	240.475	741.43	0.9850	12.7	574.94	0.6592
n-C18	C18H38	254.502	755.57	1.0432	11.9	591.45	0.6908
n-C19	C19H40	268.529	768.99	1.1014	11.2	607.44	0.7227
n-C20	C20H42	282.556	781.75	1.1597	10.5	622.95	0.7550
n-C21	C21H44	296.583	793.91	1.2181	9.9	638.02	0.7876
n-C22	C22H46	310.610	805.51	1.2766	9.4	652.67	0.8208
n-C23	C23H48	324.637	816.59	1.3351	8.8	666.94	0.8544
tricyclo-C10	C10H16	136.238	666.47	0.5040	28.0	457.27	0.3471
tricyclo-C11	C11H18	150.265	682.26	0.5651	25.2	478.67	0.4076
tricyclo-C12	C12H20	164.292	697.02	0.6267	22.9	499.06	0.4683

B.1.3 Hybrid Method

Name	molecular formula	MW	Tc (K)	Vc (m3/kmol)	ω	Method Used
C00-benzene	C6H6	78.112	562.05	0.2560	0.2103	DIPPR
C01-benzene	C7H8	92.138	591.75	0.3160	0.2640	DIPPR
C02-benzene	C8H10	106.166	623.82	0.3728	0.2991	RIAZI
C03-benzene	C9H12	120.193	647.33	0.4312	0.3485	RIAZI
C04-benzene	C10H14	134.22	666.62	0.4912	0.4056	RIAZI
C05-benzene	C11H16	148.247	683.35	0.5525	0.4673	RIAZI
C06-benzene	C12H18	162.274	698.36	0.6146	0.5320	RIAZI
C07-benzene	C13H20	176.301	712.10	0.6775	0.5991	RIAZI
C08-benzene	C14H22	190.328	724.86	0.7408	0.6683	RIAZI
C09-benzene	C15H24	204.355	736.81	0.8047	0.7396	RIAZI
C10+ benzene	C16H26	218.382	748.08	0.8689	0.8131	RIAZI
cycloaromatic-C09	C9H10	118.176	684.90	0.3960	0.3092	DIPPR
cycloaromatic-C10	C10H12	132.202	707.70	0.4364	0.3437	REGRESS
cycloaromatic-C11	C11H14	146.229	719.91	0.4924	0.3845	REGRESS
cycloaromatic-C12	C12H16	160.255	732.12	0.5484	0.4253	REGRESS
cycloaromatic-C13	C13H18	174.283	744.32	0.6044	0.4661	REGRESS
cycloaromatic-C14	C14H20	188.309	756.53	0.6604	0.5069	REGRESS
cycloaromatic-C15+	C16H24	216.362	780.95	0.7724	0.5885	REGRESS
diaromatic-C10	C10H8	128.171	748.40	0.4070	0.3020	DIPPR
diaromatic-C11	C11H10	142.195	763.71	0.4716	0.3704	REGRESS
diaromatic-C12	C12H12	156.222	772.92	0.5260	0.4132	REGRESS
diaromatic-C13	C13H14	170.249	782.13	0.5804	0.4560	REGRESS
diaromatic-C14+	C14H16	184.276	791.33	0.6348	0.4988	REGRESS
dicyclo-C08	C8H14	110.199	622.82	0.6829	0.2022	REGRESS
dicyclo-C09	C9H16	124.226	649.22	0.7779	0.2531	REGRESS

dicyclo-C10	C10H18	138.253	675.63	0.8729	0.3040	REGRESS
dicyclo-C11	C11H20	152.28	702.04	0.9679	0.3549	REGRESS
dicyclo-C12	C12H22	166.307	728.44	1.0629	0.4058	REGRESS
dicyclo-C13	C13H24	180.334	754.85	1.1579	0.4567	REGRESS
dicyclo-C14	C14H26	194.361	781.25	1.2529	0.5076	REGRESS
dicyclo-C15	C15H28	208.388	807.66	1.3479	0.5585	REGRESS
dicyclo-C16	C16H30	222.415	834.07	1.4429	0.6094	REGRESS
dicyclo-C17+	C17H32	236.442	860.47	1.5379	0.6603	REGRESS
iso-C07-	C7H16	100.202	533.05	0.4136	0.3561	RIAZI
iso-C08	C8H18	114.229	562.77	0.4695	0.3843	RIAZI
iso-C09	C9H20	128.255	589.51	0.5258	0.4136	RIAZI
iso-C10	C10H22	142.282	613.83	0.5825	0.4435	RIAZI
iso-C11	C11H24	156.308	636.15	0.6394	0.4737	RIAZI
iso-C12	C12H26	170.335	656.77	0.6965	0.5042	RIAZI
iso-C13	C13H28	184.361	675.95	0.7539	0.5348	RIAZI
iso-C14	C14H30	198.388	693.86	0.8114	0.5656	RIAZI
iso-C15	C15H32	212.415	710.67	0.8691	0.5966	RIAZI
iso-C16	C16H34	226.441	726.49	0.9270	0.6278	RIAZI
iso-C17	C17H36	240.468	741.43	0.9850	0.6592	RIAZI
iso-C18	C18H38	254.494	755.57	1.0432	0.6908	RIAZI
iso-C19	C19H40	268.521	768.99	1.1014	0.7227	RIAZI
iso-C20	C20H42	282.547	781.75	1.1597	0.7550	RIAZI
iso-C21	C21H44	296.574	793.91	1.2181	0.7876	RIAZI
iso-C22	C22H46	310.601	805.51	1.2766	0.8208	RIAZI
iso-C23	C23H48	324.627	816.59	1.3351	0.8544	RIAZI
iso-C24	C24H50	338.654	827.20	1.3938	0.8887	RIAZI
monocyclo-C07-	C7H14	98.189	565.97	0.3777	0.2447	RIAZI
monocyclo-C08	C8H16	112.216	591.40	0.4353	0.2911	RIAZI
monocyclo-C09	C9H18	126.243	614.54	0.4933	0.3362	RIAZI
monocyclo-C10	C10H20	140.27	635.81	0.5516	0.3801	RIAZI
monocyclo-C11	C11H22	154.297	655.48	0.6102	0.4233	RIAZI
monocyclo-C12	C12H24	168.324	673.78	0.6691	0.4659	RIAZI
monocyclo-C13	C13H26	182.351	690.90	0.7282	0.5081	RIAZI
monocyclo-C14	C14H28	196.378	706.97	0.7876	0.5501	RIAZI
monocyclo-C15	C15H30	210.405	722.11	0.8471	0.5919	RIAZI
monocyclo-C16	C16H32	224.432	736.42	0.9067	0.6338	RIAZI
monocyclo-C17	C17H34	238.459	749.97	0.9665	0.6759	RIAZI
monocyclo-C18	C18H36	252.486	762.84	1.0264	0.7183	RIAZI
monocyclo-C19+	C19H38	266.513	775.09	1.0865	0.7611	RIAZI
n-C07	C7H16	100.202	540.20	0.4280	0.3495	DIPPR
n-C08	C8H18	114.229	568.70	0.4860	0.3996	DIPPR

n-C09	C9H20	128.255	594.60	0.5510	0.4435	DIPPR
n-C10	C10H22	142.282	617.70	0.6170	0.4923	DIPPR
n-C11	C11H24	156.308	639.00	0.6850	0.5303	DIPPR
n-C12	C12H26	170.335	658.00	0.7550	0.5764	DIPPR
n-C13	C13H28	184.361	675.00	0.8260	0.6174	DIPPR
n-C14	C14H30	198.388	693.00	0.8970	0.6430	DIPPR
n-C15	C15H32	212.415	708.00	0.9690	0.6863	DIPPR
n-C16	C16H34	226.441	723.00	1.0400	0.7174	DIPPR
n-C17	C17H36	240.468	736.00	1.1100	0.7697	DIPPR
n-C18	C18H38	254.494	747.00	1.1900	0.8114	DIPPR
n-C19	C19H40	268.521	758.00	1.2600	0.8522	DIPPR
n-C20	C20H42	282.547	768.00	1.3400	0.9069	DIPPR
n-C21	C21H44	296.574	778.00	1.4100	0.9420	DIPPR
n-C22	C22H46	310.601	787.00	1.4800	0.9722	DIPPR
n-C23	C23H48	324.627	796.00	1.5600	1.0262	DIPPR
tricyclo-C10	C10H16	136.234	666.47	0.5040	0.3471	RIAZI
tricyclo-C11	C11H18	150.263	682.26	0.5651	0.4076	RIAZI
tricyclo-C12	C12H20	164.287	697.02	0.6267	0.4683	RIAZI

Appendix B.2 – Reference Fluid Results

In this section the first table is the reference fluids used for the density predictions, and it is followed by the reference fluid optimums.

B.2.1 DENSITY

Name	Family
Methane	n-paraffin
Ethane	n-paraffin
Propane	n-paraffin
n-butane	n-paraffin
isobutane	Iso-paraffin
cyclopentane	cyclo-paraffin
isopentane	Iso-paraffin
benzene	Alkyl-benzene
cyclohexane	cyclo-paraffin
Toluene	Alkyl-benzene
ethylcyclopentane	cyclo-paraffin
metylcyclohexane	cyclo-paraffin
ethylbenzene	Alkyl-benzene
1,1 - dimethylcyclohexane	cyclo-paraffin
ethylcyclohexane	cyclo-paraffin
iso-octane	Iso-paraffin
n-octane	n-paraffin
cumene	iso-benzene
n-propylbenzene	Alkyl-benzene
Napthalene	Napthyl
n-nonane	n-paraffin
tetralin	Napthyl
n-butylbezene	Alkyl-benzene
n-decane	n-paraffin

The data contained in the following tables is only the first 10 points of the 1656 possible points.

B.2.1.1 Numerical Regression Method

AAD	Slope	Zone Err%	Δ	Fluid #1	Fluid #2
0.325007	-0.05942	-0.02313	0.007519	Ethane	Isopentane
0.285932	-0.07268	0.035399	0.010122	Methane	Iso-octane
0.285932	-0.07324	-0.13876	0.039676	Methane	Iso-octane
0.567884	0.091402	-0.07224	0.041022	n-octane	n-propylbenzene
0.325007	-0.06096	-0.14963	0.04863	Ethane	Iso-pentane
0.609145	-0.04537	-0.08428	0.051342	Iso-butane	Methylcyclohexane
0.285932	-0.07543	-0.19446	0.055604	Methane	Iso-octane
0.285932	-0.07385	-0.19614	0.056084	Methane	Iso-octane
0.325007	-0.05806	0.213732	0.069465	Ethane	Isopentane
0.285932	-0.07447	-0.2439	0.069739	Methane	Iso-octane

B.2.1.2 Riazi/Daubert Method

AAD	Slope	Zone Err%	Δ	Fluid #1	Fluid #2
0.936668	0.016694	0.010182	0.009537	1,1-dimethyl-cyclo-hexane	n-nonane
0.658767	-0.05442	-0.016	0.010539	n-butane	benzene
0.645726	-0.0321	-0.02763	0.017841	Ethyl-benzene	n-octane
0.610676	-0.03518	-0.07724	0.047171	Ethyl-cyclo-hexane	n-octane
0.936668	0.02061	0.07377	0.069098	1,1-dimethyl-cyclo-hexane	n-nonane
0.645726	-0.02974	0.110269	0.071203	Ethyl-benzene	n-octane
0.645726	-0.03052	-0.12164	0.078547	Ethyl-benzene	n-octane
0.843254	-0.00012	-0.11167	0.094166	n-propylbenzene	n-butylbenzene
0.53205	-0.05566	0.180278	0.095917	Propane	Methylcyclohexane
1.790235	-0.06829	-0.05531	0.099012	Ethane	Cyclopentane

B.2.1.3 Hybrid Method

AAD	Slope	Zone Err%	Δ	Fluid #1	Fluid #2
1.837834	-0.12094	0.002505	0.004605	n-butane	Cumene
1.832025	-0.12027	-0.00623	0.01141	Methane	Ethane
1.912927	-0.13455	-0.01167	0.022318	Cyclopentane	Ethylbenzene
1.836722	-0.12774	-0.02499	0.045894	Benzene	Cumene
1.875889	-0.11639	-0.02606	0.048887	Methane	Isobutene
1.842415	-0.13539	-0.04419	0.081417	Cyclohexane	Ethylbenzene
1.828297	-0.11983	0.058253	0.106503	Methane	n-propylbenzene
1.837834	-0.11967	0.061226	0.112523	n-butane	Cumene
1.82813	-0.11967	0.064347	0.117634	Ethane	n-propylbenzene
1.840175	-0.11578	0.065182	0.119946	Methane	Cumene

B.2.2 VISCOSITY

B.2.2.1 Possible Reference Fluids

Name	Family
Methane	n-paraffin
Ethane	n-paraffin
Propane	n-paraffin
n-butane	n-paraffin
n-pentane	n-paraffin
Benzene	alkylbezene
n-hexane	n-paraffin
Toulene	alkylbezene
n-heptane	n-paraffin
Ethylbezene	alkylbezene
cyclooctane	cyclo-paraffin
1,1 - dimethylcyclohexane	cyclo-paraffin
ethylcyclohexane	cyclo-paraffin
iso-octane	iso-paraffin
n-octane	n-paraffin
cumene	alkylbezene
n-propylbenzene	alkylbezene
napthalene	di-aromatic
n-nonane	n-paraffin
tetralin	di-aromatic
n-butylbenzene	alkylbezene
n-decane	n-paraffin
pentamethylbenzene	alkylbezene
biphenyl	di-aromatic
n-hexylbenzene	alkylbezene
n-dodecane	n-paraffin
n-tridecane	n-paraffin
n-octylbenzene	alkylbezene
n-tetradecane	n-paraffin
n-nonylbenzene	alkylbezene
1-n-hexylnaphthalene	di-aromatic
n-pentadecane	n-paraffin
1-n-hexyl-tetralin	di-aromatic

The data contained in the following tables is only the first 10 points of the 1584 possible points.

B.2.2.2 Numerical Regression

AAD	Slope	Zone Err%	Δ	Fluid #1	Fluid #2
8.440006	4.710027	0.316297	2.669551	n-propylbenzene	n-butylbenzene
9.261202	3.597811	-0.29376	2.720553	iso-octane	n-decane
8.495148	3.176898	-0.32772	2.784007	ethylcyclohexane	n-decane
8.251813	4.735605	0.481043	3.969474	methane	n-decane
8.907528	0.723775	-0.44947	4.00363	benzene	n-decane
8.906388	3.87602	-0.50431	4.491619	benzene	cumene
20.73295	1.264132	0.342353	7.097992	benzene	n-octylbenzene
10.30734	7.247781	0.759193	7.825265	ethane	naphthalene
7.701855	1.719525	1.032894	7.955203	1,1-dimethyl-cyclohexane	n-decane
9.433799	7.141337	0.892437	8.41907	n-pentane	n-butylbenzene

B.2.2.3 Riazi/Daubert

AAD	Slope	Zone Err%	Δ	Fluid #1	Fluid #2
9.49612	1.499467	0.015178	0.144132	iso-octane	n-tridecane
8.46918	2.417631	-0.20181	1.70916	ethylbenzene	n-octane
12.58845	1.292187	0.146348	1.842299	tetralin	n-octylbenzene
8.01183	0.934215	-0.31333	2.510334	cumene	n-tridecane
18.55017	4.16454	-0.23789	4.412992	ethylcyclohexane	tetralin
8.681602	3.398274	-0.69042	5.993989	n-pentane	n-heptane
15.68409	1.763863	-0.39728	6.23105	biphenyl	n-octylbenzene
10.29058	5.383539	-0.66927	6.887165	ethane	n-propylbenzene
12.80556	1.26312	0.552826	7.079249	cumene	n-pentadecane
23.72602	0.843909	-0.32015	7.595829	n-decane	1-n-hexyl-naphthalene

B.2.2.4 Hybrid

AAD	Slope	Zone Err%	Δ	Fluid #1	Fluid #2
9.146018	1.538542	-0.03177	0.29057	cumene	n-tetradecane
8.110539	1.646828	-0.05135	0.416484	n-butylbenzene	n-decane
9.461266	6.924523	0.088627	0.838519	n-octane	n-decane
7.420455	2.211884	-0.14379	1.066983	toluene	n-decane
8.006512	3.700185	0.348216	2.787996	n-heptane	naphthalene
13.84954	1.749747	-0.22904	3.172129	cumene	n-octylbenzene
7.41359	2.709609	-0.59676	4.424169	cumene	n-decane
7.964449	3.150766	-0.56928	4.534014	n-butane	n-decane
7.864929	3.254787	-0.59146	4.651781	benzene	n-heptane
7.577006	3.262789	0.651287	4.934805	benzene	n-decane

APPENDIX C – Tables of Fuel Properties

The following appendix is filled with the experimental data that was used in these models. It is listed in tabular form, with each fuel listed in a separate table. The data includes identification number, viscosity, and density, as obtained from the CRC world fuel survey, and mole fractions of the pseudo-groups from the GCxGC.

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3896**
Fuel Type:	JP-8

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0031	0.0060

CRC Density Data						
Temperature [°C]	-36.40	-19.80	-0.20	19.50	39.70	69.50
Density [g/mL]	0.8477	0.8349	0.8197	0.8055	0.7905	0.7689

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						9.52E-05		
n = 7	4.92E-04	0.001	8.95E-04			6.72E-04		
n = 8	0.003	0.002	0.008	0.001		0.023		
n = 9	0.051	0.047	0.055	0.012		0.057	0.002	
n = 10	0.039	0.073	0.055	0.012	1.53E-04	0.041	0.008	0.002
n = 11	0.027	0.047	0.045	0.015	7.38E-04	0.024	0.019	0.006
n = 12	0.017	0.027	0.031	0.015	0.0E+00	0.015	0.020	0.008
n = 13	0.011	0.020	0.021	0.011		0.010	0.012	0.005
n = 14	0.008	0.016	0.012	0.008		0.006	0.006	0.003
n = 15	0.004	0.011	0.007	0.002		0.003	0.003	
n = 16	0.002	0.005	0.002	4.51E-04		0.001	0.002	
n = 17	8.44E-04	0.002	8.68E-04	1.07E-04				
n = 18	1.4E-04	4.43E-04	1.49E-04					
n = 19	4.17E-05	1.57E-04	4.71E-05					
n = 20	1.99E-05	3.79E-05						
n = 21	1.19E-05	1.78E-05						
n = 22	6.39E-06	8.78E-06						
n = 23	3.14E-06	2.82E-06						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.16	0.25	0.24	0.08	0.00	0.18	0.07	0.02
			0.31			0.25		
	0.73					0.27		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3897**
Fuel Type:	JP-8

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0014	0.0035	0.0073

CRC Density Data						
Temperature [°C]	-36.60	-18.80	-2.00	19.90	39.40	69.50
Density [g/mL]	0.8367	0.8225	0.8102	0.7943	0.7804	0.7586

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						1.84E-04		
n = 7	0.001	0.002	0.002			0.002		
n = 8	0.009	0.008	0.009	2.98E-04		0.013		
n = 9	0.024	0.022	0.021	0.004		0.035	0.001	
n = 10	0.039	0.046	0.035	0.007	6.94E-05	0.042	0.015	0.001
n = 11	0.042	0.060	0.047	0.012	5.91E-04	0.035	0.023	0.003
n = 12	0.034	0.061	0.037	0.009	4.63E-04	0.024	0.015	0.005
n = 13	0.026	0.055	0.024	0.006		0.011	0.009	0.002
n = 14	0.016	0.035	0.013	0.002		0.005	0.002	5.44E-04
n = 15	0.006	0.024	0.003	2.47E-04		0.002	5.89E-04	
n = 16	0.001	0.005	9.13E-04	1.85E-05		4.76E-04	0.001	
n = 17	3.77E-04	9.55E-04	2.57E-04	2.17E-05				
n = 18	9.46E-05	2.37E-04	4.59E-05					
n = 19	3.56E-05	1.05E-04	2.94E-05					
n = 20	1.7E-05	3.5E-05						
n = 21	8.29E-06	1.6E-05						
n = 22	4.71E-06	4.22E-06						
n = 23	9.56E-06	5.3E-06						
n = 24		7.26E-07						
Sub-Totals (mole frac)	0.20	0.32	0.19	0.04	0.00	0.17	0.07	0.01
			0.23			0.24		
	0.75					0.25		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3898**
Fuel Type:	JP-8

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0015	0.0038	0.0084

CRC Density Data						
Temperature [°C]	-37.00	-19.10	-0.90	18.80	39.70	69.60
Density [g/mL]	0.8525	0.8387	0.8255	0.8117	0.7963	0.7750

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	7.66E-04	0.001	0.004			0.002		
n = 8	0.006	0.005	0.012	5.09E-04		0.014		
n = 9	0.012	0.010	0.025	0.007		0.032	8.28E-04	
n = 10	0.028	0.033	0.059	0.014	5.31E-04	0.038	0.008	0.006
n = 11	0.045	0.047	0.077	0.035	0.003	0.025	0.014	0.013
n = 12	0.034	0.038	0.058	0.035	2.11E-04	0.015	0.014	0.010
n = 13	0.022	0.032	0.033	0.023		0.006	0.011	0.002
n = 14	0.011	0.027	0.013	0.012		0.003	0.003	2.86E-04
n = 15	0.002	0.011	0.003	0.002		6.61E-04	2.34E-04	
n = 16	3.52E-04	0.001	2.72E-04	4.0E-05		4.13E-05	0.006	
n = 17	5.49E-05	2.27E-04	2.17E-05	1.36E-06				
n = 18	7.89E-06	3.95E-05	1.8E-07					
n = 19	1.79E-06	2.1E-06	1.94E-06					
n = 20	6.53E-07	0.0E+00						
n = 21	0.0E+00	0.0E+00						
n = 22	0.0E+00	0.0E+00						
n = 23	0.0E+00	1.3E-06						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.16	0.21	0.29	0.13	0.00	0.14	0.06	0.03
			0.42			0.19		
	0.78					0.22		
Totals (mole frac)	1.01							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3899**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0019	0.0052	0.0125

CRC Density Data						
Temperature [°C]	-36.30	-18.70	-0.50	19.30	39.00	69.00
Density [g/mL]	0.8527	0.8386	0.8252	0.8117	0.7977	0.7765

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	2.49E-04	4.09E-04	0.001			5.75E-04		
n = 8	0.002	0.003	0.007	1.88E-04		0.003		
n = 9	0.004	0.006	0.016	0.002		0.008	3.84E-04	
n = 10	0.008	0.019	0.023	0.009	1.8E-04	0.016	0.007	0.004
n = 11	0.031	0.034	0.056	0.032	0.001	0.023	0.020	0.011
n = 12	0.042	0.062	0.066	0.035	0.0E+00	0.020	0.019	0.014
n = 13	0.032	0.057	0.045	0.021		0.011	0.016	0.007
n = 14	0.022	0.042	0.026	0.014		0.008	0.007	0.002
n = 15	0.014	0.026	0.015	0.002		0.004	0.002	
n = 16	0.004	0.008	0.003	1.95E-04		7.87E-04	0.004	
n = 17	4.51E-04	0.002	3.8E-04	2.61E-05				
n = 18	1.89E-05	2.62E-04	5.77E-06					
n = 19	1.29E-06	1.06E-05	1.99E-07					
n = 20	0.0E+00	0.0E+00						
n = 21	0.0E+00	4.14E-07						
n = 22	0.0E+00	0.0E+00						
n = 23	0.0E+00	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.16	0.26	0.26	0.12	0.00	0.09	0.08	0.04
			0.38			0.17		
	0.80					0.21		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3900**
Fuel Type:	JP-8

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0031	0.0064

CRC Density Data						
Temperature [°C]	-36.70	-22.90	-1.40	19.90	37.00	67.50
Density [g/mL]	0.8348	0.8244	0.8079	0.7924	0.7804	0.7583

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						2.87E-04		
n = 7	0.003	0.005	0.003			0.003		
n = 8	0.009	0.007	0.006	2.33E-04		0.015		
n = 9	0.031	0.019	0.022	0.005		0.063	7.36E-04	
n = 10	0.058	0.069	0.041	0.005	7.49E-05	0.052	0.005	0.002
n = 11	0.047	0.060	0.038	0.008	5.25E-04	0.029	0.009	0.007
n = 12	0.036	0.040	0.030	0.007	0.0E+00	0.018	0.010	0.010
n = 13	0.028	0.035	0.023	0.007		0.009	0.008	0.004
n = 14	0.018	0.027	0.015	0.004		0.005	0.003	9.49E-04
n = 15	0.007	0.017	0.005	3.58E-04		0.002	7.38E-04	
n = 16	0.002	0.005	0.001	2.91E-05		4.76E-04	0.002	
n = 17	4.31E-04	0.001	2.77E-04	3.42E-05				
n = 18	9.17E-05	2.25E-04	3.76E-05					
n = 19	3.22E-05	8.14E-05	1.57E-05					
n = 20	1.49E-05	2.36E-05						
n = 21	8.31E-06	9.34E-06						
n = 22	4.16E-06	2.76E-06						
n = 23	5.08E-06	6.9E-07						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.24	0.28	0.18	0.04	0.00	0.20	0.04	0.02
			0.22			0.23		
	0.74					0.26		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3901**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0018	0.0048	0.0116

CRC Density Data						
Temperature [°C]	-34.70	-17.30	0.30	19.80	39.40	69.10
Density [g/mL]	0.8528	0.8387	0.8254	0.8108	0.7970	0.7762

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						1.37E-04		
n = 7	6.17E-04	0.002	0.002			0.001		
n = 8	0.003	0.003	0.007	2.18E-04		0.006		
n = 9	0.008	0.008	0.014	0.003		0.018	5.24E-04	
n = 10	0.017	0.024	0.030	0.009	1.72E-04	0.029	0.006	0.004
n = 11	0.036	0.040	0.055	0.027	0.001	0.026	0.013	0.011
n = 12	0.038	0.051	0.058	0.027	2.07E-04	0.018	0.016	0.015
n = 13	0.030	0.045	0.039	0.020		0.010	0.015	0.007
n = 14	0.022	0.036	0.026	0.019		0.008	0.008	0.002
n = 15	0.013	0.026	0.015	0.004		0.004	0.003	
n = 16	0.004	0.009	0.003	1.31E-04		9.39E-04	0.004	
n = 17	6.28E-04	0.002	5.55E-04	4.86E-05				
n = 18	7.41E-05	4.8E-04	2.5E-05					
n = 19	1.68E-05	6.03E-05	2.51E-06					
n = 20	7.93E-06	9.09E-06						
n = 21	5.12E-06	3.08E-06						
n = 22	2.84E-06	5.94E-07						
n = 23	1.61E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.17	0.25	0.25	0.11	0.00	0.12	0.07	0.04
			0.36			0.19		
	0.78					0.23		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3902**
Fuel Type:	JP-8

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0033	0.0068

CRC Density Data						
Temperature [°C]	-37.30	-18.90	-3.10	19.50	38.80	69.50
Density [g/mL]	0.8321	0.8180	0.8066	0.7864	0.7767	0.7545

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.003	0.003	0.002			0.002		
n = 8	0.010	0.008	0.006	2.43E-04		0.012		
n = 9	0.027	0.020	0.018	0.003		0.045	6.9E-04	
n = 10	0.056	0.059	0.035	0.005	0.0E+00	0.049	0.006	7.94E-04
n = 11	0.053	0.069	0.036	0.009	4.03E-04	0.031	0.014	0.003
n = 12	0.040	0.051	0.032	0.007	0.0E+00	0.020	0.017	0.005
n = 13	0.028	0.042	0.024	0.007		0.011	0.011	0.002
n = 14	0.017	0.030	0.014	0.003		0.006	0.003	6.02E-04
n = 15	0.006	0.017	0.005	3.88E-04		0.002	6.96E-04	
n = 16	0.002	0.005	0.001	1.98E-05		6.17E-04	7.94E-04	
n = 17	5.21E-04	0.001	3.12E-04	5.83E-05				
n = 18	1.63E-04	3.9E-04	9.64E-05					
n = 19	7.13E-05	1.92E-04	6.85E-05					
n = 20	3.67E-05	8.32E-05						
n = 21	1.79E-05	4.08E-05						
n = 22	8.51E-06	1.76E-05						
n = 23	5.93E-06	6.8E-06						
n = 24		3.49E-07						
Sub-Totals (mole frac)	0.24	0.31	0.17	0.03	0.00	0.18	0.05	0.01
			0.21			0.23		
	0.76					0.24		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3938**
Fuel Type:	JP-8

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0014	0.0035	0.0073

CRC Density Data						
Temperature [°C]	-30.50	-19.40	-2.70	21.40	41.70	69.50
Density [g/mL]	0.8296	0.8209	0.8081	0.7913	0.7762	0.7563

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						9.15E-05		
n = 7	0.001	0.002	0.001			0.001		
n = 8	0.008	0.005	0.006	2.55E-04		0.010		
n = 9	0.023	0.019	0.019	0.004		0.035	0.001	
n = 10	0.042	0.044	0.037	0.006	4.05E-05	0.047	0.010	0.001
n = 11	0.053	0.066	0.047	0.012	4.61E-04	0.036	0.018	0.003
n = 12	0.043	0.062	0.041	0.008	0.0E+00	0.023	0.014	0.004
n = 13	0.030	0.055	0.023	0.007		0.011	0.009	0.002
n = 14	0.016	0.035	0.013	0.002		0.005	0.002	4.85E-04
n = 15	0.005	0.017	0.004	2.41E-04		0.002	5.98E-04	
n = 16	0.001	0.004	8.61E-04	3.02E-05		4.87E-04	0.001	
n = 17	3.75E-04	9.33E-04	2.28E-04	2.27E-05				
n = 18	9.44E-05	2.34E-04	4.95E-05					
n = 19	3.74E-05	1.11E-04	2.3E-05					
n = 20	1.74E-05	4.03E-05						
n = 21	7.53E-06	1.52E-05						
n = 22	3.23E-06	4.56E-06						
n = 23	2.76E-06	1.26E-06						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.22	0.31	0.19	0.04	0.00	0.17	0.06	0.01
			0.23			0.23		
	0.77					0.24		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3939**
Fuel Type:	JP-5

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0018	0.0052	0.0125

CRC Density Data						
Temperature [°C]	-35.30	-18.30	0.80	19.70	39.20	69.20
Density [g/mL]	0.8601	0.8463	0.8321	0.8187	0.8054	outlier

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	3.82E-04	9.11E-04	0.001			8.84E-04		
n = 8	0.003	0.002	0.005	2.84E-04		0.008		
n = 9	0.009	0.007	0.014	0.004		0.019	4.48E-04	
n = 10	0.018	0.020	0.030	0.009	1.58E-04	0.029	0.007	0.002
n = 11	0.035	0.033	0.060	0.025	0.001	0.025	0.018	0.005
n = 12	0.033	0.036	0.064	0.027	0.0E+00	0.018	0.024	0.008
n = 13	0.026	0.033	0.052	0.044		0.012	0.022	0.004
n = 14	0.020	0.031	0.038	0.022		0.010	0.010	4.71E-04
n = 15	0.011	0.023	0.018	0.004		0.004	0.001	
n = 16	9.13E-04	0.006	0.002	9.21E-05		2.09E-04	0.002	
n = 17	7.18E-05	4.51E-04	3.82E-05	4.46E-06				
n = 18	1.74E-05	2.74E-05	0.0E+00					
n = 19	9.04E-06	1.16E-05	8.72E-07					
n = 20	4.93E-06	1.96E-06						
n = 21	2.0E-06	0.0E+00						
n = 22	8.29E-07	1.23E-07						
n = 23	6.51E-07	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.16	0.19	0.29	0.14	0.00	0.13	0.08	0.02
			0.42			0.21		
	0.77					0.23		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3940**
Fuel Type:	JP-5

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0018	0.0048	0.0116

CRC Density Data						
Temperature [°C]	-29.30	-19.30	0.20	20.40	37.70	58.80
Density [g/mL]	0.8544	0.8482	0.8334	0.8192	0.8067	0.7917

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	6.13E-05	7.85E-04	2.46E-04			1.91E-04		
n = 8	8.39E-04	4.47E-04	0.002	1.69E-04		0.003		
n = 9	0.005	0.003	0.010	0.005		0.019	5.77E-04	
n = 10	0.026	0.016	0.043	0.017	2.45E-04	0.040	0.007	0.007
n = 11	0.042	0.040	0.078	0.028	0.001	0.029	0.012	0.017
n = 12	0.034	0.034	0.059	0.030	0.0E+00	0.020	0.015	0.019
n = 13	0.026	0.028	0.047	0.025		0.011	0.017	0.007
n = 14	0.017	0.028	0.030	0.012		0.008	0.007	0.003
n = 15	0.009	0.018	0.014	0.004		0.004	0.003	
n = 16	0.002	0.006	0.003	6.15E-04		0.001	0.007	
n = 17	5.64E-04	0.001	8.86E-04	1.34E-04				
n = 18	1.14E-04	4.19E-04	1.26E-04					
n = 19	2.58E-05	9.63E-05	2.58E-05					
n = 20	6.27E-06	1.33E-05						
n = 21	1.29E-06	1.01E-06						
n = 22	2.8E-07	0.0E+00						
n = 23	1.95E-07	9.72E-08						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.16	0.18	0.29	0.12	0.00	0.14	0.07	0.05
			0.41			0.20		
	0.75					0.26		
Totals (mole frac)	1.01							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3941**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0033	0.0058

CRC Density Data						
Temperature [°C]	-36.50	-18.70	0.50	20.40	40.00	70.50
Density [g/mL]	0.8405	0.8266	0.8110	0.7972	0.7831	0.7603

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.002	0.003	0.006			0.004		
n = 8	0.010	0.007	0.014	6.47E-04		0.022		
n = 9	0.024	0.018	0.031	0.010		0.055	0.001	
n = 10	0.056	0.053	0.064	0.016	2.42E-04	0.049	0.008	0.006
n = 11	0.050	0.058	0.063	0.021	0.001	0.027	0.011	0.010
n = 12	0.037	0.037	0.044	0.018	2.46E-04	0.015	0.010	0.004
n = 13	0.020	0.030	0.022	0.008		0.005	0.005	6.68E-04
n = 14	0.006	0.017	0.006	0.003		0.001	8.83E-04	1.53E-04
n = 15	0.001	0.005	0.001	3.32E-04		3.72E-04	1.52E-04	
n = 16	4.93E-04	8.8E-04	3.09E-04	3.78E-05		1.1E-04	0.006	
n = 17	1.89E-04	3.56E-04	1.32E-04	2.57E-05				
n = 18	5.84E-05	1.64E-04	2.22E-05					
n = 19	2.03E-05	5.32E-05	5.91E-06					
n = 20	9.12E-06	1.07E-05						
n = 21	4.76E-06	3.32E-06						
n = 22	3.66E-06	7.29E-07						
n = 23	5.09E-06	8.97E-07						
n = 24		2.28E-07						
Sub-Totals (mole frac)	0.21	0.23	0.25	0.08	0.00	0.18	0.04	0.02
			0.33			0.22		
	0.76					0.24		
Totals (mole frac)	1.01							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3960**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0015	0.0040	0.0087

CRC Density Data						
Temperature [°C]	-35.30	-19.60	-0.90	20.30	39.70	69.50
Density [g/mL]	0.8526	0.8410	0.8277	0.8125	0.7984	0.7773

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.001		
n = 7	0.003	0.006	0.010			0.006		
n = 8	0.009	0.008	0.015	7.26E-04		0.018		
n = 9	0.015	0.012	0.028	0.010		0.033	7.03E-04	
n = 10	0.029	0.029	0.050	0.014	1.37E-04	0.035	0.005	0.005
n = 11	0.035	0.036	0.061	0.023	9.44E-04	0.024	0.009	0.013
n = 12	0.028	0.028	0.050	0.022	0.0E+00	0.016	0.012	0.014
n = 13	0.020	0.024	0.036	0.018		0.009	0.013	0.007
n = 14	0.014	0.022	0.023	0.011		0.007	0.007	0.003
n = 15	0.008	0.014	0.014	0.003		0.004	0.003	
n = 16	0.003	0.006	0.004	4.26E-04		0.002	0.005	
n = 17	0.001	0.002	0.001	2.21E-04				
n = 18	2.25E-04	8.67E-04	2.85E-04					
n = 19	5.56E-05	2.11E-04	8.44E-05					
n = 20	1.79E-05	3.68E-05						
n = 21	6.92E-06	8.61E-06						
n = 22	3.46E-06	3.29E-07						
n = 23	8.03E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.17	0.19	0.29	0.10	0.00	0.16	0.06	0.04
			0.40			0.21		
	0.75					0.25		
Totals (mole frac)	1.01							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3961**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0016	0.0040	0.0084

CRC Density Data						
Temperature [°C]	-36.60	-18.70	-2.40	19.80	39.30	69.40
Density [g/mL]	0.8620	0.8477	0.8361	0.8201	0.8061	0.7845

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	7.17E-04	9.99E-04	0.004			0.002		
n = 8	0.008	0.010	0.023	8.72E-04		0.014		
n = 9	0.012	0.024	0.063	0.015		0.028	0.002	
n = 10	0.011	0.026	0.097	0.027	2.58E-04	0.025	0.010	2.81E-04
n = 11	0.010	0.028	0.103	0.044	0.001	0.014	0.014	1.95E-04
n = 12	0.007	0.019	0.067	0.040	0.0E+00	0.009	0.012	4.44E-04
n = 13	0.005	0.016	0.041	0.041		0.004	0.010	2.91E-04
n = 14	0.003	0.013	0.023	0.018		0.003	0.005	1.82E-04
n = 15	0.002	0.007	0.012	0.006		0.002	0.002	
n = 16	0.001	0.003	0.004	7.42E-04		5.76E-04	2.81E-04	
n = 17	6.62E-04	0.001	0.001	2.73E-04				
n = 18	2.28E-04	6.83E-04	2.71E-04					
n = 19	7.86E-05	3.08E-04	1.42E-04					
n = 20	3.26E-05	1.12E-04						
n = 21	1.0E-05	3.68E-05						
n = 22	4.22E-06	1.65E-05						
n = 23	1.12E-05	7.4E-07						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.06	0.15	0.44	0.19	0.00	0.10	0.05	0.00
			0.63			0.16		
	0.84					0.16		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3962**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0017	0.0046	0.0102

CRC Density Data						
Temperature [°C]	-36.60	-19.60	0.10	19.80	39.70	69.50
Density [g/mL]	0.8511	0.8386	0.8238	0.8097	0.7954	0.7744

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						1.98E-04		
n = 7	0.002	0.003	0.003			0.002		
n = 8	0.005	0.005	0.008	2.71E-04		0.010		
n = 9	0.013	0.011	0.016	0.003		0.030	9.81E-04	
n = 10	0.029	0.036	0.041	0.010	1.51E-04	0.037	0.007	0.003
n = 11	0.037	0.048	0.051	0.021	0.001	0.028	0.015	0.008
n = 12	0.031	0.040	0.051	0.020	0.0E+00	0.019	0.016	0.010
n = 13	0.024	0.037	0.035	0.018		0.011	0.015	0.006
n = 14	0.017	0.031	0.022	0.014		0.008	0.007	0.003
n = 15	0.011	0.022	0.013	0.004		0.005	0.003	
n = 16	0.004	0.009	0.004	1.73E-04		0.002	0.003	
n = 17	0.001	0.003	0.001	1.06E-04				
n = 18	2.2E-04	8.56E-04	1.52E-04					
n = 19	6.94E-05	2.23E-04	4.7E-05					
n = 20	2.87E-05	6.05E-05						
n = 21	1.31E-05	2.07E-05						
n = 22	6.6E-06	5.96E-06						
n = 23	6.2E-06	1.27E-06						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.17	0.25	0.24	0.09	0.00	0.15	0.07	0.03
			0.34			0.22		
	0.76					0.25		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3963**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0012	0.0029	0.0056

CRC Density Data						
Temperature [°C]	-36.50	-19.80	0.50	19.40	39.60	69.40
Density [g/mL]	0.8352	0.8222	0.8067	0.7934	0.7785	0.7569

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						3.74E-06		
n = 7	0.001	0.002	0.002			0.001		
n = 8	0.006	0.005	0.010	3.92E-04		0.011		
n = 9	0.025	0.020	0.035	0.008		0.066	0.003	
n = 10	0.078	0.079	0.078	0.016	1.24E-04	0.061	0.012	0.002
n = 11	0.040	0.080	0.049	0.013	4.96E-04	0.023	0.013	0.004
n = 12	0.023	0.034	0.027	0.010	0.0E+00	0.010	0.008	0.004
n = 13	0.016	0.021	0.018	0.006		0.005	0.005	0.002
n = 14	0.010	0.018	0.009	0.004		0.003	0.002	3.34E-04
n = 15	0.004	0.009	0.003	6.45E-04		9.05E-04	2.94E-04	
n = 16	6.28E-04	0.002	4.63E-04	3.32E-05		1.59E-04	0.002	
n = 17	1.2E-04	4.33E-04	8.34E-05	8.2E-06				
n = 18	3.02E-05	8.73E-05	1.31E-05					
n = 19	1.88E-05	3.08E-05	1.23E-05					
n = 20	1.55E-05	1.17E-05						
n = 21	1.47E-05	8.93E-06						
n = 22	1.29E-05	5.81E-06						
n = 23	1.38E-05	7.1E-06						
n = 24		4.4E-07						
Sub-Totals (mole frac)	0.20	0.27	0.23	0.06	0.00	0.18	0.05	0.01
			0.29			0.23		
	0.76					0.24		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3964**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0014	0.0037	0.0078

CRC Density Data						
Temperature [°C]	-35.90	-19.00	-1.20	19.70	39.70	69.50
Density [g/mL]	0.8439	0.8304	0.8168	0.8019	0.7876	0.7662

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						2.13E-04		
n = 7	0.002	0.003	0.004			0.002		
n = 8	0.008	0.008	0.011	3.57E-04		0.013		
n = 9	0.022	0.025	0.032	0.007		0.039	0.001	
n = 10	0.034	0.053	0.052	0.016	1.47E-04	0.038	0.008	8.94E-04
n = 11	0.033	0.053	0.053	0.022	6.91E-04	0.023	0.016	0.003
n = 12	0.026	0.038	0.043	0.017	0.0E+00	0.014	0.018	0.004
n = 13	0.019	0.032	0.027	0.017		0.009	0.011	0.002
n = 14	0.013	0.026	0.018	0.008		0.006	0.004	0.001
n = 15	0.006	0.018	0.009	0.002		0.003	0.002	
n = 16	0.002	0.007	0.003	5.6E-04		0.002	8.94E-04	
n = 17	0.001	0.003	0.001	1.93E-04				
n = 18	2.81E-04	0.001	2.59E-04					
n = 19	1.05E-04	5.41E-04	1.32E-04					
n = 20	4.24E-05	1.9E-04						
n = 21	1.69E-05	6.97E-05						
n = 22	6.17E-06	2.15E-05						
n = 23	3.78E-06	4.93E-06						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.17	0.27	0.25	0.09	0.00	0.15	0.06	0.01
			0.35			0.21		
	0.78					0.22		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3965**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0012	0.0031	0.0063

CRC Density Data						
Temperature [°C]	-38.00	-18.30	-2.30	18.80	39.60	68.90
Density [g/mL]	0.8390	0.8239	0.8123	0.7975	0.7821	0.7613

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.004	0.004	0.009			0.005		
n = 8	0.014	0.011	0.018	7.95E-04		0.021		
n = 9	0.033	0.023	0.039	0.010		0.049	6.49E-04	
n = 10	0.050	0.059	0.059	0.010	1.17E-04	0.036	0.004	0.004
n = 11	0.039	0.047	0.050	0.015	6.17E-04	0.020	0.007	0.010
n = 12	0.029	0.029	0.040	0.016	0.0E+00	0.012	0.009	0.009
n = 13	0.021	0.025	0.028	0.012		0.006	0.008	0.003
n = 14	0.012	0.023	0.015	0.007		0.004	0.003	9.03E-04
n = 15	0.005	0.012	0.006	0.001		0.001	8.75E-04	
n = 16	0.001	0.003	0.001	1.53E-04		4.06E-04	0.004	
n = 17	3.37E-04	8.44E-04	2.95E-04	5.85E-05				
n = 18	5.26E-05	2.18E-04	2.97E-05					
n = 19	9.77E-06	4.73E-05	3.09E-06					
n = 20	2.62E-06	2.75E-06						
n = 21	8.12E-07	0.0E+00						
n = 22	1.37E-07	2.7E-07						
n = 23	1.66E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.21	0.24	0.27	0.07	0.00	0.15	0.04	0.03
			0.34			0.19		
	0.79					0.22		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3966**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0031	0.0060

CRC Density Data						
Temperature [°C]	-35.50	-20.00	0.40	19.20	39.70	69.40
Density [g/mL]	0.8366	0.8243	0.8085	0.7954	0.7801	0.7587

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.002	0.002	0.006			0.003		
n = 8	0.014	0.009	0.020	8.9E-04		0.029		
n = 9	0.038	0.036	0.046	0.012		0.055	0.001	
n = 10	0.039	0.063	0.053	0.009	9.6E-05	0.041	0.006	0.003
n = 11	0.034	0.052	0.043	0.013	7.29E-04	0.023	0.010	0.007
n = 12	0.026	0.036	0.031	0.013	5.49E-04	0.013	0.011	0.007
n = 13	0.019	0.028	0.024	0.008		0.007	0.008	0.002
n = 14	0.013	0.022	0.013	0.005		0.004	0.003	8.56E-04
n = 15	0.005	0.012	0.005	6.55E-04		0.001	7.51E-04	
n = 16	0.001	0.003	0.001	1.27E-04		5.03E-04	0.003	
n = 17	4.15E-04	9.57E-04	3.81E-04	1.27E-04				
n = 18	1.33E-04	4.41E-04	8.47E-05					
n = 19	4.72E-05	1.39E-04	4.31E-05					
n = 20	1.94E-05	3.38E-05						
n = 21	7.48E-06	1.04E-05						
n = 22	3.33E-06	2.3E-06						
n = 23	1.99E-06	3.1E-07						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.19	0.26	0.24	0.06	0.00	0.18	0.04	0.02
			0.31			0.22		
	0.76					0.24		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3967**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0031	0.0060

CRC Density Data						
Temperature [°C]	-37.70	-19.50	0.10	19.90	39.70	69.50
Density [g/mL]	0.8381	0.8244	0.8095	0.7955	0.7811	0.7596

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.003	0.004	0.005			0.003		
n = 8	0.011	0.010	0.017	6.52E-04		0.020		
n = 9	0.027	0.032	0.043	0.010		0.047	0.002	
n = 10	0.037	0.061	0.059	0.017	1.49E-04	0.041	0.009	0.002
n = 11	0.034	0.058	0.053	0.016	6.71E-04	0.024	0.014	0.004
n = 12	0.025	0.039	0.038	0.013	3.14E-04	0.014	0.012	0.005
n = 13	0.018	0.032	0.025	0.009		0.008	0.007	0.002
n = 14	0.011	0.023	0.013	0.004		0.004	0.002	6.25E-04
n = 15	0.004	0.012	0.004	6.69E-04		0.001	6.5E-04	
n = 16	9.11E-04	0.003	8.74E-04	9.56E-05		3.81E-04	0.002	
n = 17	2.6E-04	7.72E-04	2.34E-04	3.04E-05				
n = 18	4.54E-05	1.9E-04	2.38E-05					
n = 19	1.21E-05	5.25E-05	5.29E-05					
n = 20	4.36E-06	8.45E-06						
n = 21	1.84E-06	1.04E-06						
n = 22	1.03E-06	1.79E-06						
n = 23	0.0E+00	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.17	0.28	0.26	0.07	0.00	0.16	0.05	0.01
			0.33			0.21		
	0.78					0.22		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3968**
Fuel Type:	JP-8

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0014	0.0033	0.0070

CRC Density Data						
Temperature [°C]	-34.80	-17.80	1.10	20.60	40.50	68.70
Density [g/mL]	0.8361	0.8228	0.8089	0.7952	0.7806	0.7609

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						3.62E-04		
n = 7	0.002	0.003	0.003			0.003		
n = 8	0.006	0.005	0.007	3.11E-04		0.017		
n = 9	0.024	0.017	0.024	0.005		0.046	6.19E-04	
n = 10	0.041	0.044	0.045	0.008	6.47E-04	0.045	0.006	0.003
n = 11	0.061	0.063	0.054	0.018	0.003	0.029	0.012	0.007
n = 12	0.047	0.054	0.040	0.014	2.41E-04	0.016	0.012	0.007
n = 13	0.026	0.039	0.023	0.008		0.007	0.007	0.003
n = 14	0.013	0.024	0.010	0.005		0.004	0.003	0.001
n = 15	0.005	0.011	0.005	7.94E-04		0.001	0.001	
n = 16	0.002	0.003	0.001	1.49E-04		5.73E-04	0.003	
n = 17	6.54E-04	0.001	4.18E-04	4.25E-05				
n = 18	1.7E-04	4.48E-04	8.13E-05					
n = 19	6.16E-05	1.37E-04	4.12E-05					
n = 20	2.72E-05	3.53E-05						
n = 21	1.26E-05	1.22E-05						
n = 22	6.3E-06	2.18E-06						
n = 23	4.4E-06	9.84E-07						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.23	0.27	0.21	0.06	0.00	0.17	0.04	0.02
			0.27			0.21		
	0.77					0.23		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3969**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0011	0.0029	0.0059

CRC Density Data						
Temperature [°C]	-37.10	-17.80	0.50	19.50	39.70	69.50
Density [g/mL]	0.8343	0.8194	0.8057	0.7929	0.7776	0.7559

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.002	0.004	0.009			0.003		
n = 8	0.018	0.010	0.026	0.001		0.031		
n = 9	0.036	0.032	0.038	0.010		0.050	7.66E-04	
n = 10	0.054	0.057	0.046	0.012	3.06E-04	0.038	0.004	0.004
n = 11	0.052	0.053	0.039	0.016	0.002	0.021	0.006	0.010
n = 12	0.037	0.034	0.024	0.017	0.0E+00	0.010	0.008	0.010
n = 13	0.025	0.025	0.014	0.010		0.004	0.007	0.003
n = 14	0.015	0.020	0.007	0.008		0.003	0.003	0.001
n = 15	0.006	0.011	0.003	0.001		9.41E-04	6.86E-04	
n = 16	0.001	0.002	5.25E-04	8.44E-05		1.97E-04	0.004	
n = 17	4.2E-04	5.74E-04	1.02E-04	1.54E-05				
n = 18	8.13E-05	1.84E-04	1.4E-05					
n = 19	1.92E-05	2.61E-05	6.26E-07					
n = 20	4.93E-06	3.41E-06						
n = 21	1.62E-06	1.77E-07						
n = 22	7.95E-07	0.0E+00						
n = 23	2.04E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.25	0.25	0.21	0.07	0.00	0.16	0.03	0.03
			0.28			0.20		
	0.78					0.23		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**3970**
Fuel Type:	JP-8

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0014	0.0036	0.0078

CRC Density Data						
Temperature [°C]	-38.80	-18.90	0.40	19.80	39.50	61.80
Density [g/mL]	0.8422	0.8269	0.8131	0.7994	0.7855	0.7702

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.003	0.004	0.003			0.002		
n = 8	0.008	0.007	0.007	2.78E-04		0.012		
n = 9	0.019	0.017	0.019	0.004		0.041	6.58E-04	
n = 10	0.039	0.048	0.037	0.007	5.05E-05	0.049	0.006	0.001
n = 11	0.043	0.061	0.047	0.013	6.44E-04	0.034	0.013	0.005
n = 12	0.029	0.051	0.041	0.011	2.86E-04	0.021	0.015	0.007
n = 13	0.020	0.041	0.029	0.010		0.011	0.012	0.004
n = 14	0.017	0.032	0.017	0.007		0.007	0.005	0.002
n = 15	0.007	0.021	0.008	0.001		0.003	0.002	
n = 16	0.002	0.007	0.003	8.81E-05		0.001	0.001	
n = 17	7.24E-04	0.002	6.98E-04	4.52E-05				
n = 18	1.79E-04	7.4E-04	1.43E-04					
n = 19	5.46E-05	1.98E-04	5.45E-05					
n = 20	2.49E-05	5.2E-05						
n = 21	1.44E-05	2.23E-05						
n = 22	8.79E-06	1.04E-05						
n = 23	5.11E-06	5.18E-06						
n = 24		3.33E-07						
Sub-Totals (mole frac)	0.19	0.29	0.21	0.05	0.00	0.18	0.06	0.02
			0.27			0.24		
	0.75					0.26		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4108**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0015	0.0037	0.0079

CRC Density Data						
Temperature [°C]	-34.70	-18.00	0.70	20.00	39.40	68.80
Density [g/mL]	0.8473	0.8343	0.8201	0.8061	0.7919	0.7709

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.002	0.002	0.006			0.003		
n = 8	0.009	0.010	0.019	6.07E-04		0.015		
n = 9	0.020	0.038	0.051	0.010		0.032	0.002	
n = 10	0.023	0.050	0.057	0.019	2.01E-04	0.026	0.013	0.002
n = 11	0.022	0.042	0.059	0.019	9.8E-04	0.019	0.017	0.006
n = 12	0.017	0.032	0.040	0.016	0.0E+00	0.014	0.012	0.007
n = 13	0.013	0.028	0.028	0.014		0.008	0.011	0.004
n = 14	0.010	0.022	0.018	0.009		0.006	0.005	0.003
n = 15	0.007	0.017	0.011	0.003		0.004	0.004	
n = 16	0.004	0.010	0.005	3.73E-04		0.003	0.002	
n = 17	0.003	0.006	0.002	1.42E-04				
n = 18	7.27E-04	0.003	6.27E-04					
n = 19	1.7E-04	0.001	1.9E-04					
n = 20	3.59E-05	1.99E-04						
n = 21	9.69E-06	2.87E-05						
n = 22	3.18E-06	1.71E-06						
n = 23	1.48E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.13	0.26	0.30	0.09	0.00	0.13	0.07	0.02
			0.39			0.20		
	0.78					0.22		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4109**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0016	0.0044	0.0100

CRC Density Data						
Temperature [°C]	-31.20	-19.10	-0.20	19.60	39.30	68.80
Density [g/mL]	0.8463	0.8365	0.8224	0.8083	0.7942	0.7735

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	8.47E-04	0.002	0.002			0.001		
n = 8	0.004	0.004	0.006	3.21E-04		0.010		
n = 9	0.015	0.011	0.020	0.007		0.032	7.98E-04	
n = 10	0.030	0.037	0.045	0.012	1.78E-04	0.035	0.006	0.003
n = 11	0.039	0.046	0.053	0.023	0.001	0.026	0.013	0.009
n = 12	0.036	0.038	0.048	0.022	0.0E+00	0.017	0.016	0.010
n = 13	0.027	0.036	0.034	0.017		0.009	0.014	0.005
n = 14	0.018	0.030	0.020	0.014		0.007	0.006	0.003
n = 15	0.009	0.020	0.011	0.003		0.004	0.003	
n = 16	0.004	0.007	0.004	5.06E-04		0.002	0.003	
n = 17	0.001	0.003	0.002	2.46E-04				
n = 18	3.9E-04	0.001	4.36E-04					
n = 19	1.3E-04	4.31E-04	1.85E-04					
n = 20	4.59E-05	1.08E-04						
n = 21	1.55E-05	2.91E-05						
n = 22	6.9E-06	6.44E-06						
n = 23	9.61E-06	2.5E-06						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.19	0.24	0.25	0.10	0.00	0.14	0.06	0.03
			0.35			0.21		
	0.77					0.24		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4110**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0014	0.0034	0.0072

CRC Density Data						
Temperature [°C]	-35.00	-18.40	-0.40	19.80	39.60	69.40
Density [g/mL]	0.8402	0.8272	0.8135	0.7992	0.7848	0.7636

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.002	0.003	0.003			0.002		
n = 8	0.009	0.007	0.009	4.09E-04		0.016		
n = 9	0.031	0.023	0.028	0.007		0.048	8.46E-04	
n = 10	0.044	0.059	0.050	0.010	1.05E-04	0.044	0.006	0.002
n = 11	0.040	0.054	0.048	0.015	7.31E-04	0.027	0.011	0.006
n = 12	0.030	0.037	0.041	0.017	5.07E-04	0.016	0.013	0.008
n = 13	0.021	0.031	0.028	0.010		0.008	0.011	0.003
n = 14	0.013	0.024	0.016	0.007		0.005	0.004	0.001
n = 15	0.006	0.015	0.007	0.001		0.002	0.001	
n = 16	0.002	0.005	0.002	9.97E-05		9.05E-04	0.002	
n = 17	7.07E-04	0.002	6.91E-04	1.06E-04				
n = 18	1.67E-04	6.71E-04	1.37E-04					
n = 19	4.72E-05	1.77E-04	4.16E-05					
n = 20	1.59E-05	3.89E-05						
n = 21	6.02E-06	8.68E-06						
n = 22	2.68E-06	8.32E-07						
n = 23	4.87E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.20	0.26	0.23	0.07	0.00	0.17	0.05	0.02
			0.30			0.22		
	0.76					0.24		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4111**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0015	0.0041	0.0089

CRC Density Data						
Temperature [°C]	-34.40	-19.60	-0.20	19.70	39.30	68.80
Density [g/mL]	0.8480	0.8362	0.8216	0.8072	0.7931	0.7713

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.002	0.003	0.008			0.004		
n = 8	0.009	0.009	0.012	4.34E-04		0.017		
n = 9	0.018	0.018	0.022	0.006		0.041	0.001	
n = 10	0.038	0.050	0.045	0.012	2.08E-04	0.035	0.007	0.003
n = 11	0.036	0.050	0.041	0.020	0.002	0.021	0.013	0.008
n = 12	0.029	0.034	0.034	0.021	7.42E-04	0.014	0.013	0.010
n = 13	0.022	0.030	0.023	0.016		0.007	0.012	0.006
n = 14	0.016	0.025	0.015	0.017		0.005	0.007	0.005
n = 15	0.010	0.018	0.009	0.005		0.004	0.004	
n = 16	0.005	0.008	0.004	6.92E-04		0.003	0.003	
n = 17	0.003	0.005	0.002	2.86E-04				
n = 18	5.12E-04	0.002	3.21E-04					
n = 19	8.46E-05	4.19E-04	5.24E-05					
n = 20	1.92E-05	5.5E-05						
n = 21	7.38E-06	7.19E-06						
n = 22	4.02E-06	9.85E-07						
n = 23	4.22E-06	1.11E-07						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.19	0.25	0.22	0.10	0.00	0.15	0.06	0.03
			0.32			0.21		
	0.76					0.24		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4152**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0012	0.0027	0.0055

CRC Density Data						
Temperature [°C]	-36.70	-19.40	0.00	19.60	39.70	69.50
Density [g/mL]	0.8297	0.8160	0.8012	0.7873	0.7723	0.7507

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.003	0.005	0.008			0.004		
n = 8	0.012	0.009	0.013	5.34E-04		0.026		
n = 9	0.040	0.025	0.031	0.009		0.067	7.46E-04	
n = 10	0.068	0.060	0.047	0.009	3.76E-04	0.039	0.003	0.006
n = 11	0.065	0.056	0.036	0.015	0.002	0.020	0.005	0.012
n = 12	0.051	0.035	0.024	0.014	0.0E+00	0.010	0.007	0.008
n = 13	0.034	0.027	0.014	0.008		0.003	0.005	0.001
n = 14	0.013	0.022	0.005	0.005		0.001	0.001	1.77E-04
n = 15	0.003	0.007	0.001	3.76E-04		2.33E-04	8.15E-05	
n = 16	3.67E-04	5.83E-04	8.56E-05	1.07E-05		8.53E-06	0.006	
n = 17	7.18E-05	1.12E-04	1.08E-05	0.0E+00				
n = 18	1.42E-05	4.84E-05	0.0E+00					
n = 19	3.77E-06	3.31E-06	5.59E-07					
n = 20	1.48E-06	1.41E-07						
n = 21	1.08E-06	0.0E+00						
n = 22	4.25E-07	0.0E+00						
n = 23	9.77E-07	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.29	0.25	0.18	0.06	0.00	0.17	0.03	0.03
			0.24			0.20		
	0.78					0.23		
Totals (mole frac)	1.01							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4154**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0012	0.0028	0.0055

CRC Density Data						
Temperature [°C]	-34.30	-19.80	0.00	19.50	39.70	69.50
Density [g/mL]	0.8243	0.8126	0.7970	0.7831	0.7681	0.7465

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.002	0.003	0.003			0.002		
n = 8	0.015	0.010	0.012	4.17E-04		0.019		
n = 9	0.053	0.037	0.039	0.009		0.055	9.23E-04	
n = 10	0.068	0.079	0.050	0.010	8.23E-05	0.044	0.005	9.79E-04
n = 11	0.053	0.062	0.042	0.012	4.85E-04	0.024	0.009	0.002
n = 12	0.036	0.040	0.029	0.009	2.58E-04	0.013	0.007	0.002
n = 13	0.019	0.028	0.018	0.005		0.005	0.005	0.001
n = 14	0.008	0.016	0.008	0.002		0.003	0.001	3.74E-04
n = 15	0.003	0.008	0.003	3.46E-04		0.001	3.2E-04	
n = 16	9.16E-04	0.003	8.24E-04	9.24E-05		3.55E-04	9.79E-04	
n = 17	3.1E-04	0.001	2.63E-04	5.03E-05				
n = 18	8.38E-05	3.5E-04	6.51E-05					
n = 19	2.73E-05	1.44E-04	3.4E-05					
n = 20	8.85E-06	3.71E-05						
n = 21	3.24E-06	5.58E-06						
n = 22	1.36E-06	1.21E-07						
n = 23	1.42E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.26	0.29	0.20	0.05	0.00	0.17	0.03	0.01
			0.25			0.20		
	0.80					0.20		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4156**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0031	0.0061

CRC Density Data						
Temperature [°C]	-30.90	-17.30	-0.10	19.90	39.50	69.30
Density [g/mL]	0.8267	0.8157	0.8027	0.7883	0.7738	0.7528

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.004	0.006	0.013			0.003		
n = 8	0.011	0.009	0.017	5.34E-04		0.014		
n = 9	0.024	0.014	0.025	0.009		0.036	0.001	
n = 10	0.066	0.047	0.047	0.018	4.04E-04	0.038	0.008	0.006
n = 11	0.0E+00	0.064	0.050	0.022	0.002	0.023	0.011	0.012
n = 12	0.058	0.114	0.032	0.022	0.0E+00	0.012	0.009	0.006
n = 13	0.033	0.035	0.017	0.007		0.003	0.005	8.86E-04
n = 14	0.009	0.019	0.005	0.003		9.31E-04	7.24E-04	1.18E-04
n = 15	0.001	0.005	6.88E-04	2.39E-04		1.37E-04	4.43E-05	
n = 16	2.24E-04	4.02E-04	6.19E-05	3.89E-06		1.54E-06	0.006	
n = 17	4.3E-05	6.05E-05	4.17E-06	4.87E-07				
n = 18	8.57E-06	1.38E-05	0.0E+00					
n = 19	2.65E-06	1.37E-06	0.0E+00					
n = 20	8.95E-07	0.0E+00						
n = 21	3.19E-07	0.0E+00						
n = 22	0.0E+00	0.0E+00						
n = 23	0.0E+00	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.21	0.31	0.21	0.08	0.00	0.13	0.04	0.03
			0.29			0.17		
	0.81					0.20		
Totals (mole frac)	1.01							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4157**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0015	0.0040	0.0089

CRC Density Data						
Temperature [°C]	-37.20	-19.20	-1.40	19.50	39.70	69.50
Density [g/mL]	0.8126	0.7996	0.7863	0.7719	0.7575	0.7367

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						1.33E-06		
n = 7	3.92E-04	5.79E-04	5.63E-05			9.34E-05		
n = 8	9.86E-04	5.91E-04	3.7E-04	3.33E-06		2.96E-04		
n = 9	0.004	0.001	0.002	3.63E-04		0.003	0.003	
n = 10	0.043	0.023	0.010	0.002	0.0E+00	0.011	0.010	4.63E-05
n = 11	0.054	0.166	0.004	0.0E+00	0.0E+00	0.009	0.007	8.02E-05
n = 12	0.024	0.392	0.002	1.14E-05	0.0E+00	0.005	0.007	2.14E-04
n = 13	0.014	0.120	0.004	8.8E-05		0.003	0.005	2.31E-04
n = 14	0.007	0.031	0.004	2.6E-05		0.002	0.003	3.91E-05
n = 15	0.004	0.009	0.002	3.73E-05		9.61E-04	3.61E-04	
n = 16	2.34E-04	0.002	1.7E-04	3.45E-06		8.66E-05	4.63E-05	
n = 17	4.36E-05	3.99E-04	6.1E-05	1.06E-05				
n = 18	1.2E-05	1.59E-04	6.83E-05					
n = 19	2.82E-06	5.0E-05	8.2E-05					
n = 20	4.85E-07	1.5E-05						
n = 21	0.0E+00	4.67E-06						
n = 22	8.32E-07	5.84E-06						
n = 23	1.73E-06	1.45E-06						
n = 24		1.76E-07						
Sub-Totals (mole frac)	0.15	0.75	0.03	0.00	0.00	0.04	0.03	0.00
			0.03			0.07		
	0.93					0.07		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4158**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0014	0.0035	0.0074

CRC Density Data						
Temperature [°C]	-34.20	-21.30	-0.40	19.70	39.50	69.50
Density [g/mL]	0.8235	0.8136	0.7974	0.7835	0.7693	0.7480

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						3.37E-06		
n = 7	8.9E-04	6.56E-04	0.001			0.001		
n = 8	0.005	0.003	0.004	1.95E-04		0.006		
n = 9	0.014	0.010	0.012	0.003		0.030	6.21E-04	
n = 10	0.046	0.067	0.029	0.003	1.97E-04	0.033	0.003	0.001
n = 11	0.034	0.195	0.020	0.009	6.44E-04	0.019	0.005	0.004
n = 12	0.027	0.151	0.014	0.008	0.0E+00	0.012	0.007	0.005
n = 13	0.019	0.074	0.016	0.007		0.006	0.007	0.002
n = 14	0.010	0.029	0.010	0.004		0.003	0.002	3.53E-04
n = 15	0.003	0.011	0.004	8.24E-04		9.85E-04	3.4E-04	
n = 16	6.23E-04	0.002	5.39E-04	2.35E-05		1.58E-04	0.001	
n = 17	1.26E-04	5.29E-04	9.06E-05	1.43E-05				
n = 18	3.52E-05	1.42E-04	1.05E-05					
n = 19	1.6E-05	5.69E-05	6.02E-06					
n = 20	1.02E-05	2.21E-05						
n = 21	6.58E-06	9.54E-06						
n = 22	4.44E-06	2.34E-06						
n = 23	5.07E-06	9.58E-07						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.16	0.54	0.11	0.04	0.00	0.11	0.03	0.01
			0.15			0.14		
	0.85					0.15		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4159**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0011	0.0023	0.0046

CRC Density Data						
Temperature [°C]	-29.20	-17.70	0.10	19.60	39.50	69.50
Density [g/mL]	0.8295	0.8200	0.8062	0.7922	0.7775	0.7555

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						1.91E-06		
n = 7	2.69E-05	5.31E-04	7.33E-05			5.81E-05		
n = 8	0.003	2.52E-04	0.005	5.02E-04		0.026		
n = 9	0.109	0.018	0.054	0.022		0.068	0.013	
n = 10	0.0E+00	0.029	0.059	0.027	0.0E+00	0.042	0.034	9.98E-05
n = 11	0.0E+00	0.111	0.039	0.028	9.85E-05	0.020	0.032	1.78E-04
n = 12	0.057	0.086	0.022	0.015	0.0E+00	0.012	0.011	3.69E-04
n = 13	0.024	0.010	0.009	0.003		0.003	0.001	0.0E+00
n = 14	2.09E-04	0.005	6.75E-04	1.43E-04		5.93E-05	0.0E+00	1.53E-06
n = 15	2.41E-06	1.74E-04	0.0E+00	1.43E-07		2.92E-06	3.85E-06	
n = 16	5.36E-07	0.0E+00	1.88E-07	5.14E-07		1.13E-06	9.98E-05	
n = 17	0.0E+00	1.57E-07	0.0E+00	1.08E-06				
n = 18	0.0E+00	1.19E-07	5.96E-07					
n = 19	0.0E+00	0.0E+00	2.46E-06					
n = 20	0.0E+00	1.23E-07						
n = 21	0.0E+00	0.0E+00						
n = 22	0.0E+00	0.0E+00						
n = 23	7.59E-07	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.19	0.26	0.19	0.10	0.00	0.17	0.09	0.00
			0.28			0.26		
	0.74					0.26		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4195**
Fuel Type:	JP-8

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0018	0.0050	0.0116

CRC Density Data						
Temperature [°C]	-31.30	-18.40	0.00	19.90	39.70	69.40
Density [g/mL]	0.8462	0.8360	0.8222	0.8078	0.7934	0.7727

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	3.93E-04	7.64E-04	0.001			6.51E-04		
n = 8	0.002	0.002	0.004	2.26E-04		0.005		
n = 9	0.007	0.007	0.012	0.003		0.020	3.13E-04	
n = 10	0.022	0.027	0.041	0.009	3.25E-04	0.032	0.002	0.004
n = 11	0.039	0.054	0.064	0.021	0.002	0.025	0.006	0.009
n = 12	0.034	0.051	0.062	0.023	2.87E-04	0.018	0.009	0.011
n = 13	0.024	0.046	0.045	0.018		0.009	0.011	0.006
n = 14	0.016	0.037	0.030	0.012		0.007	0.006	0.004
n = 15	0.009	0.024	0.017	0.004		0.004	0.004	
n = 16	0.004	0.010	0.007	4.14E-04		0.003	0.004	
n = 17	0.002	0.004	0.003	2.98E-04				
n = 18	4.33E-04	0.002	7.04E-04					
n = 19	1.16E-04	5.46E-04	2.95E-04					
n = 20	4.21E-05	1.34E-04						
n = 21	1.17E-05	3.07E-05						
n = 22	4.12E-06	5.26E-06						
n = 23	9.72E-06	8.9E-07						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.16	0.27	0.29	0.09	0.00	0.12	0.04	0.03
			0.38			0.16		
	0.81					0.20		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4197**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0029	0.0056

CRC Density Data						
Temperature [°C]	-36.70	-19.20	0.10	20.00	39.70	69.60
Density [g/mL]	0.8396	0.8267	0.8118	0.7974	0.7829	0.7615

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.004	0.004	0.007			0.004		
n = 8	0.012	0.011	0.017	5.78E-04		0.024		
n = 9	0.028	0.032	0.038	0.009		0.052	0.003	
n = 10	0.036	0.058	0.049	0.013	8.25E-05	0.043	0.012	0.002
n = 11	0.034	0.054	0.046	0.014	5.51E-04	0.025	0.016	0.005
n = 12	0.027	0.037	0.036	0.012	0.0E+00	0.015	0.013	0.006
n = 13	0.019	0.030	0.026	0.009		0.008	0.009	0.002
n = 14	0.012	0.023	0.014	0.005		0.005	0.003	7.85E-04
n = 15	0.005	0.013	0.006	5.45E-04		0.002	7.79E-04	
n = 16	0.001	0.004	0.001	9.05E-05		4.55E-04	0.002	
n = 17	2.54E-04	9.73E-04	2.34E-04	4.64E-05				
n = 18	4.8E-05	2.33E-04	3.25E-05					
n = 19	1.07E-05	4.94E-05	3.05E-06					
n = 20	3.33E-06	6.92E-06						
n = 21	1.41E-06	5.41E-07						
n = 22	6.22E-07	0.0E+00						
n = 23	1.79E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.18	0.27	0.24	0.06	0.00	0.18	0.06	0.02
			0.30			0.24		
	0.75					0.25		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4198**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0012	0.0029	0.0054

CRC Density Data						
Temperature [°C]	-35.20	-19.20	-0.90	19.60	39.60	69.40
Density [g/mL]	0.8391	0.8263	0.8125	0.7975	0.7829	0.7612

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.002	0.004	0.004			0.002		
n = 8	0.010	0.010	0.012	7.09E-04		0.020		
n = 9	0.041	0.029	0.048	0.014		0.070	0.001	
n = 10	0.047	0.083	0.070	0.016	1.62E-04	0.045	0.006	9.06E-04
n = 11	0.017	0.056	0.051	0.016	7.43E-04	0.022	0.011	0.002
n = 12	0.012	0.032	0.037	0.016	0.0E+00	0.013	0.012	0.003
n = 13	0.008	0.027	0.025	0.010		0.006	0.008	0.001
n = 14	0.009	0.021	0.011	0.006		0.003	0.002	3.99E-04
n = 15	0.003	0.010	0.004	0.001		9.87E-04	5.01E-04	
n = 16	7.19E-04	0.002	6.44E-04	6.02E-05		2.76E-04	9.06E-04	
n = 17	2.26E-04	5.33E-04	2.29E-04	5.42E-05				
n = 18	9.35E-05	2.4E-04	6.33E-05					
n = 19	5.74E-05	1.04E-04	7.33E-05					
n = 20	3.95E-05	4.69E-05						
n = 21	2.66E-05	3.23E-05						
n = 22	1.66E-05	1.69E-05						
n = 23	1.09E-05	8.8E-06						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.15	0.27	0.26	0.08	0.00	0.18	0.04	0.01
			0.34			0.22		
	0.77					0.23		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4324**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0029	0.0055

CRC Density Data						
Temperature [°C]	-36.80	-16.70	3.30	18.30	39.40	62.60
Density [g/mL]	0.8352	0.8190	0.8041	0.7940	0.7781	0.7616

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.003	0.005	0.006			0.003		
n = 8	0.011	0.009	0.013	4.79E-04		0.018		
n = 9	0.029	0.025	0.032	0.006		0.050	9.55E-04	
n = 10	0.054	0.063	0.053	0.010	8.13E-05	0.044	0.005	0.003
n = 11	0.044	0.061	0.047	0.012	5.09E-04	0.024	0.008	0.007
n = 12	0.032	0.040	0.039	0.011	5.77E-04	0.014	0.009	0.007
n = 13	0.021	0.032	0.025	0.008		0.007	0.007	0.003
n = 14	0.012	0.023	0.014	0.005		0.004	0.002	8.44E-04
n = 15	0.005	0.013	0.006	8.0E-04		0.002	8.43E-04	
n = 16	0.001	0.004	0.001	1.39E-04		5.48E-04	0.003	
n = 17	5.13E-04	0.002	4.33E-04	4.15E-05				
n = 18	8.52E-05	5.19E-04	7.87E-05					
n = 19	2.25E-05	1.77E-04	2.69E-05					
n = 20	8.37E-06	3.45E-05						
n = 21	3.7E-06	7.47E-06						
n = 22	2.13E-06	9.56E-07						
n = 23	2.46E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.21	0.28	0.24	0.05	0.00	0.17	0.04	0.02
			0.29			0.20		
	0.78					0.22		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4325**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0015	0.0041	0.0074

CRC Density Data						
Temperature [°C]	-35.20	-17.30	1.30	29.20	40.70	69.10
Density [g/mL]	0.8452	0.8309	0.8173	0.7978	0.7896	0.7693

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						2.9E-04		
n = 7	0.002	0.004	0.003			0.002		
n = 8	0.006	0.006	0.008	2.84E-04		0.014		
n = 9	0.018	0.016	0.022	0.005		0.042	0.001	
n = 10	0.038	0.047	0.042	0.010	1.65E-04	0.041	0.008	0.003
n = 11	0.038	0.052	0.049	0.016	9.01E-04	0.027	0.014	0.008
n = 12	0.033	0.042	0.043	0.014	0.0E+00	0.018	0.014	0.010
n = 13	0.024	0.036	0.029	0.016		0.009	0.012	0.005
n = 14	0.016	0.029	0.018	0.009		0.006	0.005	0.003
n = 15	0.009	0.018	0.010	0.002		0.004	0.003	
n = 16	0.004	0.007	0.003	1.75E-04		0.002	0.003	
n = 17	0.001	0.003	0.001	1.43E-04				
n = 18	3.29E-04	9.78E-04	2.09E-04					
n = 19	1.01E-04	3.06E-04	9.5E-05					
n = 20	3.64E-05	7.07E-05						
n = 21	1.44E-05	2.47E-05						
n = 22	6.78E-06	8.33E-06						
n = 23	6.82E-06	3.21E-06						
n = 24		1.99E-07						
Sub-Totals (mole frac)	0.19	0.26	0.23	0.07	0.00	0.16	0.06	0.03
			0.30			0.22		
	0.75					0.25		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4326**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0015	0.0035	0.0077

CRC Density Data						
Temperature [°C]	-34.70	-18.90	-1.30	19.30	39.50	62.30
Density [g/mL]	0.8451	0.8323	0.8190	0.8043	0.7897	0.7736

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						2.46E-04		
n = 7	0.001	0.003	0.003			0.003		
n = 8	0.006	0.006	0.009	3.08E-04		0.014		
n = 9	0.018	0.016	0.022	0.006		0.042	0.001	
n = 10	0.035	0.047	0.043	0.010	1.45E-04	0.041	0.008	0.003
n = 11	0.039	0.053	0.047	0.017	9.01E-04	0.027	0.014	0.008
n = 12	0.034	0.041	0.045	0.014	0.0E+00	0.018	0.015	0.010
n = 13	0.025	0.037	0.029	0.014		0.009	0.012	0.005
n = 14	0.017	0.029	0.017	0.008		0.006	0.005	0.003
n = 15	0.009	0.017	0.010	0.002		0.004	0.003	
n = 16	0.004	0.007	0.003	1.53E-04		0.002	0.003	
n = 17	0.001	0.003	0.001	1.44E-04				
n = 18	3.36E-04	0.001	2.3E-04					
n = 19	9.51E-05	2.97E-04	7.1E-05					
n = 20	3.17E-05	6.48E-05						
n = 21	1.2E-05	1.99E-05						
n = 22	5.22E-06	3.86E-06						
n = 23	2.71E-06	2.86E-07						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.19	0.26	0.23	0.07	0.00	0.16	0.06	0.03
			0.30			0.22		
	0.75					0.25		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4327**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0016	0.0041	0.0095

CRC Density Data						
Temperature [°C]	-34.90	-18.90	4.80	22.30	39.60	69.40
Density [g/mL]	0.8572	0.8441	0.8268	0.8144	0.8017	0.7805

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	6.47E-05	2.54E-04	6.1E-04			5.98E-04		
n = 8	0.003	0.002	0.005	1.98E-04		0.005		
n = 9	0.006	0.005	0.013	0.003		0.020	0.001	
n = 10	0.028	0.020	0.053	0.013	1.05E-04	0.051	0.009	0.003
n = 11	0.035	0.055	0.073	0.022	8.83E-04	0.033	0.015	0.009
n = 12	0.027	0.036	0.062	0.017	0.0E+00	0.023	0.017	0.013
n = 13	0.021	0.032	0.042	0.018		0.013	0.017	0.007
n = 14	0.014	0.026	0.026	0.008		0.009	0.008	0.004
n = 15	0.008	0.018	0.013	0.003		0.005	0.004	
n = 16	0.003	0.007	0.004	2.26E-04		0.002	0.003	
n = 17	8.97E-04	0.002	0.001	1.37E-04				
n = 18	1.55E-04	7.03E-04	1.79E-04					
n = 19	2.58E-05	1.54E-04	2.36E-05					
n = 20	4.93E-06	1.56E-05						
n = 21	5.34E-07	3.73E-07						
n = 22	0.0E+00	0.0E+00						
n = 23	3.81E-07	3.23E-07						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.15	0.20	0.29	0.08	0.00	0.16	0.07	0.04
			0.38			0.24		
	0.73					0.27		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4363**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0012	0.0028	0.0051

CRC Density Data						
Temperature [°C]	-38.20	-19.60	-0.40	19.50	39.70	69.50
Density [g/mL]	0.8322	0.8174	0.8028	0.7889	0.7742	0.7525

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.002	0.003	0.005			0.002		
n = 8	0.013	0.008	0.015	6.49E-04		0.032		
n = 9	0.043	0.039	0.038	0.009		0.054	9.29E-04	
n = 10	0.052	0.063	0.047	0.009	6.57E-05	0.044	0.005	0.002
n = 11	0.046	0.057	0.044	0.012	4.92E-04	0.025	0.008	0.005
n = 12	0.033	0.040	0.031	0.009	0.0E+00	0.014	0.008	0.005
n = 13	0.020	0.030	0.022	0.005		0.006	0.006	0.002
n = 14	0.011	0.020	0.011	0.003		0.003	0.002	6.45E-04
n = 15	0.005	0.011	0.004	4.74E-04		0.001	6.52E-04	
n = 16	0.001	0.004	0.001	1.34E-04		4.88E-04	0.002	
n = 17	4.21E-04	0.002	3.87E-04	4.17E-05				
n = 18	6.28E-05	6.23E-04	4.89E-05					
n = 19	1.32E-05	1.42E-04	6.1E-06					
n = 20	5.73E-06	2.68E-05						
n = 21	2.62E-06	5.7E-06						
n = 22	1.26E-06	1.33E-07						
n = 23	1.2E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.23	0.28	0.22	0.05	0.00	0.18	0.03	0.01
			0.27			0.22		
	0.77					0.23		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4364**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0017	0.0044	0.0105

CRC Density Data						
Temperature [°C]	-33.80	-17.20	0.10	19.30	39.30	69.00
Density [g/mL]	0.8564	0.8435	0.8309	0.8172	0.8027	0.7816

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						1.54E-06		
n = 7	9.96E-07	2.94E-04	6.22E-05			2.26E-05		
n = 8	5.42E-05	7.33E-05	1.66E-04	3.49E-05		4.59E-04		
n = 9	0.003	6.05E-04	0.006	0.002		0.020	0.001	
n = 10	0.035	0.022	0.056	0.014	1.42E-04	0.047	0.013	6.97E-04
n = 11	0.055	0.059	0.081	0.023	9.16E-04	0.030	0.029	0.003
n = 12	0.029	0.041	0.052	0.017	0.0E+00	0.017	0.027	0.006
n = 13	0.015	0.026	0.033	0.017		0.009	0.018	0.005
n = 14	0.011	0.029	0.022	0.009		0.008	0.009	0.005
n = 15	0.007	0.015	0.016	0.003		0.006	0.006	
n = 16	0.004	0.008	0.008	3.99E-04		0.005	6.97E-04	
n = 17	0.002	0.004	0.004	4.76E-04				
n = 18	4.7E-04	0.002	0.001					
n = 19	1.63E-04	6.8E-04	6.39E-04					
n = 20	6.45E-05	1.97E-04						
n = 21	2.31E-05	6.06E-05						
n = 22	8.74E-06	1.45E-05						
n = 23	6.79E-06	3.17E-06						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.16	0.21	0.28	0.09	0.00	0.14	0.10	0.02
			0.37			0.24		
	0.74					0.26		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4365**
Fuel Type:	Jet A

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0030	0.0060

CRC Density Data						
Temperature [°C]	-33.20	-16.50	-0.40	21.30	39.50	69.50
Density [g/mL]	0.8342	0.8210	0.8075	0.7923	0.7791	0.7575

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.001	0.001	0.003			0.002		
n = 8	0.007	0.005	0.010	5.17E-04		0.014		
n = 9	0.023	0.016	0.028	0.007		0.042	6.36E-04	
n = 10	0.053	0.048	0.055	0.011	7.04E-05	0.044	0.005	0.005
n = 11	0.057	0.061	0.060	0.018	6.21E-04	0.028	0.009	0.012
n = 12	0.046	0.045	0.051	0.017	0.0E+00	0.017	0.011	0.006
n = 13	0.029	0.039	0.031	0.009		0.007	0.006	9.12E-04
n = 14	0.009	0.024	0.010	0.002		0.002	7.4E-04	8.06E-05
n = 15	0.001	0.007	0.002	1.36E-04		2.25E-04	2.71E-05	
n = 16	1.23E-04	5.71E-04	7.65E-05	6.72E-06		7.87E-06	0.005	
n = 17	1.25E-05	4.91E-05	1.72E-06	0.0E+00				
n = 18	2.0E-06	3.87E-06	0.0E+00					
n = 19	1.06E-06	3.54E-07	2.4E-05					
n = 20	2.74E-07	0.0E+00						
n = 21	0.0E+00	0.0E+00						
n = 22	0.0E+00	0.0E+00						
n = 23	0.0E+00	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.23	0.25	0.25	0.06	0.00	0.16	0.04	0.02
			0.32			0.19		
	0.79					0.22		
Totals (mole frac)	1.01							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4366**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0016	0.0039	0.0083

CRC Density Data						
Temperature [°C]	-36.70	-19.00	0.60	21.40	35.80	69.20
Density [g/mL]	0.8497	0.8359	0.8221	0.8076	0.7972	0.7733

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.003	0.003	0.006			0.003		
n = 8	0.008	0.010	0.013	3.99E-04		0.010		
n = 9	0.011	0.010	0.022	0.005		0.023	5.11E-04	
n = 10	0.020	0.022	0.035	0.009	0.0E+00	0.045	0.007	0.001
n = 11	0.049	0.035	0.070	0.023	5.53E-04	0.028	0.020	0.004
n = 12	0.038	0.036	0.062	0.022	0.0E+00	0.016	0.029	0.006
n = 13	0.028	0.034	0.046	0.017		0.009	0.020	0.003
n = 14	0.016	0.031	0.023	0.006		0.006	0.005	0.002
n = 15	0.006	0.015	0.008	0.001		0.002	0.002	
n = 16	0.002	0.004	0.002	1.69E-04		9.72E-04	0.001	
n = 17	9.04E-04	0.002	0.001	2.37E-04				
n = 18	3.35E-04	8.61E-04	3.25E-04					
n = 19	1.45E-04	3.81E-04	1.92E-04					
n = 20	6.96E-05	1.21E-04						
n = 21	2.68E-05	4.54E-05						
n = 22	9.16E-06	7.19E-06						
n = 23	8.82E-05	1.09E-06						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.18	0.20	0.29	0.08	0.00	0.14	0.08	0.02
			0.37			0.23		
	0.76					0.24		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4368**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0024	0.0024	0.0051

CRC Density Data						
Temperature [°C]	-37.50	-19.50	-0.20	19.60	39.70	69.60
Density [g/mL]	0.8274	0.8130	0.7982	0.7843	0.7696	0.7482

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						2.65E-04		
n = 7	0.004	0.006	0.002			0.002		
n = 8	0.011	0.008	0.006	2.21E-04		0.012		
n = 9	0.032	0.020	0.021	0.004		0.068	0.001	
n = 10	0.081	0.089	0.050	0.007	0.0E+00	0.067	0.006	0.001
n = 11	0.063	0.084	0.044	0.009	2.58E-04	0.035	0.009	0.002
n = 12	0.036	0.050	0.029	0.007	0.0E+00	0.016	0.007	0.002
n = 13	0.014	0.028	0.014	0.004		0.004	0.004	5.81E-04
n = 14	0.005	0.011	0.005	0.003		0.002	0.001	1.11E-04
n = 15	0.002	0.004	0.002	4.67E-04		6.38E-04	1.85E-04	
n = 16	3.6E-04	9.16E-04	4.15E-04	6.7E-05		1.13E-04	0.001	
n = 17	5.98E-05	2.11E-04	6.61E-05	1.2E-05				
n = 18	1.01E-05	4.96E-05	2.91E-06					
n = 19	3.08E-06	8.09E-06	4.48E-06					
n = 20	1.08E-06	7.46E-07						
n = 21	5.62E-07	1.59E-07						
n = 22	2.38E-07	0.0E+00						
n = 23	2.02E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.25	0.30	0.17	0.03	0.00	0.21	0.03	0.01
			0.21			0.24		
	0.76					0.24		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4369**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0033	0.0058

CRC Density Data						
Temperature [°C]	-37.90	-19.40	-0.20	20.90	39.60	69.50
Density [g/mL]	0.8500	0.8351	0.8206	0.8056	0.7919	0.7704

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.001	0.002	0.005			0.002		
n = 8	0.007	0.006	0.015	8.4E-04		0.009		
n = 9	0.014	0.014	0.038	0.016		0.037	0.001	
n = 10	0.037	0.045	0.096	0.040	2.0E-04	0.053	0.008	0.004
n = 11	0.036	0.059	0.095	0.039	8.86E-04	0.028	0.011	0.006
n = 12	0.021	0.032	0.050	0.026	0.0E+00	0.012	0.010	0.004
n = 13	0.009	0.021	0.021	0.011		0.004	0.006	0.001
n = 14	0.004	0.014	0.007	0.004		0.002	0.002	3.48E-04
n = 15	0.001	0.005	0.002	7.45E-04		6.55E-04	3.25E-04	
n = 16	4.09E-04	0.001	5.52E-04	7.36E-05		1.48E-04	0.004	
n = 17	9.87E-05	3.92E-04	1.45E-04	2.03E-05				
n = 18	2.33E-05	1.77E-04	1.14E-05					
n = 19	5.15E-06	2.88E-05	2.06E-06					
n = 20	1.46E-06	1.91E-06						
n = 21	2.32E-07	0.0E+00						
n = 22	1.37E-07	0.0E+00						
n = 23	1.18E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.13	0.20	0.33	0.14	0.00	0.15	0.04	0.02
			0.47			0.19		
	0.80					0.20		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4370**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0015	0.0039	0.0083

CRC Density Data						
Temperature [°C]	-38.00	-20.00	-0.60	19.40	39.50	69.40
Density [g/mL]	0.8531	0.8391	0.8250	0.8110	0.7965	0.7754

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						3.96E-04		
n = 7	0.002	0.005	0.005			0.003		
n = 8	0.006	0.007	0.014	4.0E-04		0.012		
n = 9	0.013	0.017	0.031	0.008		0.032	0.002	
n = 10	0.025	0.039	0.050	0.013	1.44E-04	0.036	0.013	0.002
n = 11	0.032	0.040	0.060	0.019	7.46E-04	0.023	0.021	0.006
n = 12	0.025	0.032	0.046	0.016	0.0E+00	0.016	0.020	0.008
n = 13	0.019	0.027	0.034	0.014		0.009	0.015	0.005
n = 14	0.014	0.026	0.022	0.009		0.006	0.006	0.004
n = 15	0.008	0.018	0.012	0.002		0.004	0.005	
n = 16	0.005	0.009	0.005	4.54E-04		0.003	0.002	
n = 17	0.003	0.005	0.003	2.34E-04				
n = 18	8.58E-04	0.002	7.48E-04					
n = 19	2.44E-04	0.001	2.78E-04					
n = 20	5.79E-05	2.32E-04						
n = 21	1.42E-05	4.06E-05						
n = 22	4.32E-06	4.88E-06						
n = 23	2.05E-05	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.15	0.23	0.28	0.08	0.00	0.15	0.08	0.02
			0.37			0.23		
	0.75					0.25		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4371**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0012	0.0029	0.0057

CRC Density Data						
Temperature [°C]	-31.50	-19.90	-0.70	19.50	39.50	69.20
Density [g/mL]	0.8251	0.8160	0.8014	0.7871	0.7725	0.7510

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						3.05E-04		
n = 7	0.004	0.005	0.003			0.003		
n = 8	0.011	0.008	0.007	2.82E-04		0.015		
n = 9	0.036	0.019	0.023	0.004		0.067	8.51E-04	
n = 10	0.067	0.069	0.040	0.006	9.12E-05	0.054	0.005	0.002
n = 11	0.055	0.060	0.034	0.009	5.2E-04	0.028	0.008	0.006
n = 12	0.042	0.042	0.029	0.007	0.0E+00	0.016	0.009	0.008
n = 13	0.032	0.035	0.021	0.004		0.008	0.007	0.002
n = 14	0.018	0.026	0.011	0.002		0.004	0.002	2.14E-04
n = 15	0.004	0.013	0.003	1.36E-04		8.23E-04	1.34E-04	
n = 16	4.77E-04	0.002	2.1E-04	5.28E-06		6.1E-05	0.002	
n = 17	6.23E-05	2.19E-04	1.28E-05	9.43E-07				
n = 18	7.5E-06	1.83E-05	8.92E-07					
n = 19	1.71E-06	2.56E-06	5.19E-07					
n = 20	1.66E-07	0.0E+00						
n = 21	0.0E+00	0.0E+00						
n = 22	0.0E+00	0.0E+00						
n = 23	4.23E-07	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.27	0.28	0.17	0.03	0.00	0.20	0.03	0.02
			0.20			0.23		
	0.75					0.25		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4384**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0032	0.0061

CRC Density Data						
Temperature [°C]	-37.70	-19.20	-0.10	19.60	39.80	69.80
Density [g/mL]	0.8357	0.8209	0.8063	0.7925	0.7779	0.7565

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.003	0.004	0.003			0.002		
n = 8	0.009	0.007	0.008	3.13E-04		0.012		
n = 9	0.032	0.021	0.025	0.006		0.049	7.94E-04	
n = 10	0.054	0.062	0.043	0.007	2.51E-05	0.046	0.005	0.002
n = 11	0.047	0.058	0.040	0.010	3.48E-04	0.028	0.009	0.006
n = 12	0.037	0.041	0.035	0.009	0.0E+00	0.017	0.009	0.009
n = 13	0.028	0.036	0.025	0.008		0.010	0.010	0.004
n = 14	0.019	0.028	0.015	0.003		0.006	0.003	0.002
n = 15	0.008	0.018	0.006	4.58E-04		0.003	0.001	
n = 16	0.002	0.006	0.001	3.41E-05		7.33E-04	0.002	
n = 17	5.77E-04	0.002	3.51E-04	2.65E-05				
n = 18	9.25E-05	2.86E-04	4.41E-05					
n = 19	2.05E-05	8.28E-05	1.02E-05					
n = 20	5.34E-06	1.15E-05						
n = 21	1.39E-06	3.31E-07						
n = 22	2.15E-07	0.0E+00						
n = 23	3.18E-06	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.24	0.28	0.20	0.04	0.00	0.17	0.04	0.02
			0.25			0.21		
	0.77					0.23		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4385**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0013	0.0027	0.0054

CRC Density Data						
Temperature [°C]	-37.70	-19.60	-0.20	19.70	39.70	69.70
Density [g/mL]	0.8396	0.8250	0.8104	0.7964	0.7818	0.7601

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.002	0.003	0.006			0.003		
n = 8	0.010	0.008	0.015	7.26E-04		0.016		
n = 9	0.024	0.018	0.034	0.011		0.045	0.001	
n = 10	0.052	0.050	0.068	0.017	1.67E-04	0.048	0.007	0.005
n = 11	0.050	0.060	0.069	0.024	8.66E-04	0.029	0.011	0.009
n = 12	0.037	0.038	0.048	0.019	9.75E-04	0.016	0.010	0.004
n = 13	0.019	0.028	0.023	0.008		0.005	0.005	6.19E-04
n = 14	0.005	0.018	0.006	0.002		0.001	7.47E-04	9.27E-05
n = 15	0.001	0.004	0.001	1.3E-04		3.3E-04	8.31E-05	
n = 16	2.27E-04	6.02E-04	1.74E-04	1.66E-05		6.53E-05	0.005	
n = 17	8.01E-05	1.76E-04	5.87E-05	6.44E-06				
n = 18	3.39E-05	7.29E-05	1.72E-05					
n = 19	2.0E-05	4.11E-05	1.71E-05					
n = 20	1.41E-05	1.66E-05						
n = 21	1.04E-05	7.84E-06						
n = 22	8.48E-06	4.42E-06						
n = 23	1.85E-05	3.16E-06						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.20	0.23	0.27	0.08	0.00	0.16	0.04	0.02
			0.35			0.20		
	0.78					0.22		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4386**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0015	0.0036	0.0076

CRC Density Data						
Temperature [°C]	-38.20	-19.50	-0.10	19.70	39.70	69.70
Density [g/mL]	0.8515	0.8367	0.8224	0.8086	0.7941	0.7729

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						0.0E+00		
n = 7	0.001	0.003	0.005			8.71E-04		
n = 8	0.005	0.006	0.012	4.26E-04		0.005		
n = 9	0.014	0.012	0.047	0.009		0.029	5.01E-04	
n = 10	0.025	0.047	0.101	0.014	3.94E-04	0.025	0.004	0.002
n = 11	0.023	0.041	0.080	0.031	0.002	0.016	0.009	0.004
n = 12	0.019	0.026	0.059	0.034	0.0E+00	0.010	0.013	0.005
n = 13	0.015	0.027	0.045	0.032		0.007	0.011	0.001
n = 14	0.010	0.031	0.024	0.014		0.004	0.003	1.87E-04
n = 15	0.003	0.017	0.006	0.001		8.95E-04	3.61E-04	
n = 16	4.49E-04	0.002	7.24E-04	1.5E-04		1.43E-04	0.002	
n = 17	1.23E-04	4.27E-04	2.09E-04	5.66E-05				
n = 18	3.82E-05	1.9E-04	3.12E-05					
n = 19	9.67E-06	5.63E-05	3.99E-06					
n = 20	2.78E-06	7.35E-06						
n = 21	1.01E-06	1.39E-07						
n = 22	1.8E-07	0.0E+00						
n = 23	9.17E-07	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.12	0.21	0.38	0.14	0.00	0.10	0.04	0.01
			0.52			0.14		
	0.85					0.15		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4433**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0015	0.0035	0.0069

CRC Density Data						
Temperature [°C]	-38.10	-19.70	-0.30	19.50	39.70	69.60
Density [g/mL]	0.8564	0.8417	0.8275	0.8135	0.7988	0.7775

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						2.53E-04		
n = 7	0.002	0.003	0.002			0.002		
n = 8	0.007	0.006	0.024	5.86E-04		0.011		
n = 9	0.018	0.038	0.088	0.017		0.020	0.002	
n = 10	0.013	0.042	0.104	0.036	2.75E-04	0.017	0.006	2.32E-04
n = 11	0.010	0.031	0.076	0.041	0.001	0.012	0.009	6.81E-04
n = 12	0.007	0.021	0.053	0.026	3.32E-04	0.012	0.010	0.002
n = 13	0.005	0.018	0.034	0.022		0.010	0.010	0.002
n = 14	0.004	0.012	0.020	0.012		0.007	0.008	0.003
n = 15	0.002	0.005	0.013	0.004		0.006	0.008	
n = 16	0.002	0.003	0.007	8.48E-04		0.004	2.32E-04	
n = 17	7.08E-04	0.002	0.003	5.17E-04				
n = 18	1.59E-04	6.36E-04	7.8E-04					
n = 19	3.11E-05	2.63E-04	1.11E-04					
n = 20	4.25E-06	4.29E-05						
n = 21	7.98E-07	8.04E-07						
n = 22	0.0E+00	0.0E+00						
n = 23	0.0E+00	0.0E+00						
n = 24		0.0E+00						
Sub-Totals (mole frac)	0.07	0.18	0.42	0.16	0.00	0.10	0.05	0.01
			0.59			0.15		
	0.84					0.16		
Totals (mole frac)	1.00							

APPENDIX C. Tables of Fuel Properties

Fuel Description	
POSF No.:	**4461**
Fuel Type:	Jet A-1

CRC Viscosity Data			
Temperature [°C]	20	-20	-40
Viscosity [Pa·s]	0.0012	0.0026	0.0052

CRC Density Data						
Temperature [°C]	-38.10	-19.60	-0.20	19.60	39.70	69.80
Density [g/mL]	0.8352	0.8205	0.8058	0.7919	0.7772	0.7559

Detailed Hydrocarbon Type

	Saturates (mole frac)					**Aromatics (mole frac)**		
	n- Paraffins	*iso*- Paraffins	*cyclo*- Paraffins			Benzenes		Diaromatics
			Mono-	Di-	Tri-	Alkyl-	Cyclo-	
Carbon No.	C_nH_{2n+2}	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}	C_nH_{2n-4}	C_nH_{2n-6}	C_nH_{2n-8}	
n = 6						4.17E-06		
n = 7	9.98E-04	0.001	0.002			0.001		
n = 8	0.013	0.009	0.013	5.3E-04		0.025		
n = 9	0.033	0.035	0.036	0.008		0.065	0.002	
n = 10	0.051	0.068	0.049	0.010	6.79E-05	0.052	0.011	0.002
n = 11	0.046	0.066	0.047	0.012	4.33E-04	0.025	0.015	0.003
n = 12	0.030	0.044	0.031	0.009	0.0E+00	0.012	0.010	0.003
n = 13	0.017	0.029	0.018	0.005		0.005	0.006	0.001
n = 14	0.009	0.018	0.008	0.003		0.002	0.002	0.001
n = 15	0.004	0.009	0.004	6.36E-04		0.001	0.001	
n = 16	0.002	0.003	0.001	5.54E-05		9.9E-04	0.002	
n = 17	8.6E-04	0.002	7.06E-04	9.49E-05				
n = 18	3.04E-04	7.55E-04	2.28E-04					
n = 19	1.29E-04	3.64E-04	2.22E-04					
n = 20	7.27E-05	1.59E-04						
n = 21	4.67E-05	9.04E-05						
n = 22	3.21E-05	5.36E-05						
n = 23	2.32E-05	3.34E-05						
n = 24		2.86E-06						
Sub-Totals (mole frac)	0.21	0.29	0.21	0.05	0.00	0.19	0.05	0.01
			0.26			0.24		
	0.75					0.25		
Totals (mole frac)	1.00							

APPENDIX D – MATLAB Code

Appendix D.1 – Density Algorithm Code

```
%% INFORMATION
%
%  Combined GCSP program from the previous programs in order to graph the
%  data for reporting and presentations. It is also useful for spotting
%  coding errors and logic fallacies.
%
%  Matt Evanhoe, UDRI
%
%  The Calculation contained are based upon theory (mostly Teja and Rice) and
%  regression from other work done to compile this program.

%% DATA IMPORT AND CLEANING
clear all; close all; clc;

%Import all Information
builder_t = xlsread('builder.csv');
psuedo_group = xlsread('psuedo group original.csv');
ref_fluids = xlsread('ref fluids.csv');
crcden = xlsread('crc2.csv');

%Matrix Sizing
[c,~] = size(psuedo_group);
[~,b] = size(ref_fluids);
[m,n] = size(builder_t);

%Removing Header from Samples
builder_nam = zeros(1,n);
builder_num = zeros(m-1,n);
for j = 2:m
    for i = 1:n
        builder_nam(i) = builder_t(1,i);
```

```
        builder_num(j-1, i) = builder_t(j,i);
    end
end
clear i j builder_t;
[m,n] = size(builder_num);

%Data File Cleaning
builder_temp = zeros(c,n);
for i = 1:n
    for j = 1:m
        if 33 >= j
            builder_temp(j,i) = builder_num(j,i);
        elseif j >= 34 && 49 >= j
            builder_temp(j+1,i) = builder_num(j,i) + builder_num(j+18,i);
        elseif j == 50
            builder_temp(51, i) = builder_num(j,i);
        elseif j == 51
            builder_temp(34, i) = builder_num(j,i);
        elseif j > 51 && j < 68

        elseif j >= 68 && j < 98
            builder_temp(j-16, i) = builder_num(j,i);
        elseif j == 98

        elseif j == 99
            builder_temp(j-17, i) = builder_num(j,i);
        elseif j == 100
            builder_temp(j-17, i) = builder_num(100, i) + builder_num(101,i);
        elseif j == 101

        else
            builder_temp(j-18, i) = builder_num(j,i);
        end
    end
end
builder_num = builder_temp;
clear m builder_temp;

%Pseudo-Critcial Values
num_comp = length(builder_num);
Mm = zeros(1,n);
acc = zeros(1,n);
Zcm = zeros(1,n);
mole_frac = zeros(num_comp, n);
for i = 1:n
```

```
   [Mm(i), ~, acc(i), Zcm(i), mole_frac(:,i), ~] = molecalc(builder_num(:,i).',
psuedo_group, num_comp);
end
clear builder_num

Vcm = zeros(1,n);
Vcm2 = zeros(1,n);
Tcm = zeros(1,n);
em = zeros(1,n);
kays_vcm = zeros(1,n);
kays_vcm2 = zeros(1,n);
kays_tcm = zeros(1,n);
for i = 1:n
   [Vcm(i), Tcm(i), em(i), ~, ~, ~] = rice_pseudocrit_simple(mole_frac(:,i).',
psuedo_group, num_comp, Mm(i), 0); %aij = 1
   Vcm2(i) = ((Vcm(i)*10^3)/Mm(i))^-1;

end
clear mole_frac psuedo_group num_comp

%%  DENSITY
t_C = zeros(n,6);
t_K = zeros(n,6);

for i = 1:n
   t_C(i,1) = crcden(i,3);
   t_C(i,2) = crcden(i,5);
   t_C(i,3) = crcden(i,7);
   t_C(i,4) = crcden(i,9);
   t_C(i,5) = crcden(i,11);
   t_C(i,6) = crcden(i,13);
   t_K(i,:) = t_C(i,:) + 273.15;
end
[~,f] = size(t_C);
clear t_C

runner = xlsread('runner.csv');
for k = 1:length(runner)

%Density - Teja & Rice - 1978'ish
rice_temp1 = runner(k,1); %n-octane
rice_temp2 = runner(k,2); %n-propylbenzene
rice_temp3 = 152; %n-decane
rice_temp4 = 1; %METHANE
rice_ref1 = zeros(1,b);
rice_ref2 = zeros(1,b);
```

```
rice_ref3 = zeros(1,b);
rice_ref4 = zeros(1,b);
for i=1:b
   rice_ref1(i) = ref_fluids(rice_temp1,i);
   rice_ref2(i) = ref_fluids(rice_temp2,i);
   rice_ref3(i) = ref_fluids(rice_temp3,i);
   rice_ref4(i) = ref_fluids(rice_temp4,i);
end
clear rice_temp1 rice_temp2 rice_temp3 rice_temp4;

t_Rden = zeros(n,f);
t_R2 = zeros(n,f);

delta_w = zeros(1,n);
pred_den_rice = zeros(n,f);
slope = zeros(n,f);
den_err_act = zeros(n,f);
pred_den_lk = zeros(n,f);
pred_den_cout = zeros(n,f);
pred_den_red = zeros(n,f);
pred_den_kays = zeros(n,f);
kays_red = zeros(n,f);
den_storage = zeros(n,f);

for i = 1:n
   for j = 1:f
      t_Rden(i,j) = t_K(i,j)/Tcm(i);

      %Teja & Rice Method
      delta_w(i) = (acc(i)-rice_ref1(6))/(rice_ref2(6)-rice_ref1(6));
      [pred_den_rice(i,j), slope(i,j)] = rice_pred_den2(t_Rden(i,j), rice_ref1, rice_ref2,
Vcm(i), Mm(i), delta_w(i));
      den_err_act(i,j) = ((crcden(i,2*j)-pred_den_rice(i,j))/pred_den_rice(i,j))*100;

      %Coutinho Method
      pred_den_cout(i,j) = cout_pred_den(t_Rden(i,j), ref_fluids(4,:), ref_fluids(10,:),
ref_fluids(227,:), Vcm(i), Mm(i), acc(i));
      err_cout(i,j) = ((crcden(i,2*j)-pred_den_cout(i,j))/pred_den_cout(i,j))*100;
      pred_den_red3(i,j) = pred_den_cout(i,j)/Vcm2(i);

      %Reduced based on T-R Method
      pred_den_red(i,j) = pred_den_rice(i,j)/Vcm2(i);

      den_storage(i,j) = crcden(i,2*j);
   end
end
```

```
%AAD
point_err  = mean(mean(den_err_act));
ave_err(:,k) = mean(den_err_act);
ave_errb = mean(mean(err_cout));
for i = 1:n
   for j = 1:f
      aad_sing(i,j) = abs(den_err_act(i,j)- point_err);
      aad_cout_a(i,j) = abs(err_cout(i,j) - ave_errb);
   end
end
aad_cout = sum(sum(aad_cout_a))/(n*f);


aad(k) = sum(sum(aad_sing))/(n*f);
slope_std = std(slope);
slope = mean(slope);
clear aad_sing

slope_out(:,k) = slope';
std_out(:, k) = slope_std';
end

root = -0.05;
l=1;
y=1;
for i = 1:length(runner)
   for j = 1:6
      plotter(l, :) = [aad(i), slope_out(j,i), ave_err(j,i), abs(aad(i)*ave_err(j,i)), i];

      t1 = slope_out(j,i);
      if t1 > (1.1*root) && t1 < (0.9*root)
         pairs(y, :) = [aad(i), slope_out(j,i), ave_err(j,i), i];
         y= y+1;
      else

      end
      l = l+1;
   end
end


crc_red = den_storage(40,3)/Vcm2(40);
crc_red2 = den_storage(40,3)/kays_vcm2(40);

[den_num, den_name] = xlsread('denlist.csv');
```

```
qq = length(den_num);
for i = 1:qq
   ref(i,:) = ref_fluids(den_num(i), :);
   [ref_den(i), red_den(i)] = den_calc(t_Rden(40,3), ref(i,:));
end
clear ref_fluids

%Regression Lines
x = linspace(-10,15);
aad_line = polyfit(plotter(:,2), plotter(:,1), 2);
ave_line = polyfit(plotter(:,2), plotter(:,3), 1);


%% PLOTS

%Info for xy-line
xyx = linspace(-10,10);
xyx25up = 0.975*xyx;
xyx25down = 1.025*xyx;

%Density Plots
crcden_store = zeros(n,f);
temp_store = zeros(n,f);
for i = 1:n
   for j = 1:f
   crcden_store(i,j) = crcden(i,2*j);
   temp_store(i,j) = crcden(i,(2*j +1));
   end
end

den1 = reshape(pred_den_rice,1,n*f);
den2 = reshape(pred_den_lk,1,n*f);
den3 = reshape(pred_den_cout,1,n*f);
den4 = reshape(pred_den_kays,1,n*f);
crc1 = reshape(crcden_store,1,n*f);
%clear crcden_store

%Teja/Rice
figure(1)
hold on
scatter(crc1, den1, 5, 'b', 'MarkerFaceColor', 'b')
plot(xyx, xyx25up, 'k--')
plot(xyx, xyx25down, 'k--')
plot(xyx,xyx)

box
```

```
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
axis([0.7 0.95 0.7 0.95])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('CRC Density Values')
ylabel('Model Predicted Values')
legend('Model A', '2.5% Error Lines', 'Location', 'SouthEast')
title('Teja/Rice')
hold off

%Coutinho
figure(2)
hold on
scatter(crc1, den3, 5, 'b', 'MarkerFaceColor', 'b')
plot(xyx, xyx25up, 'k--')
plot(xyx, xyx25down, 'k--')
plot(xyx,xyx)

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
axis([0.7 0.95 0.7 0.95])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('CRC Density Values')
ylabel('Model Predicted Values')
legend('Prediction', '2.5% Error Lines', 'Location', 'SouthEast')
hold off

figure(3)
hold on
scatter(ref(:,6), red_den)
scatter(acc(40), pred_den_red(40,3), 'r')
scatter(acc(40), crc_red, 'rd')
hold off

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('Acentric Factor')
ylabel('Reduced Density [g/cm^3]')
legend('Reference Fluids', 'Teja-Rice', 'CRC - Teja-Rice', 'Location', 'SouthEast')
hold off

figure(4)
hold on
scatter(plotter(:,2), plotter(:,1))
scatter(plotter(:,2), plotter(:,3))
plot(x, polyval(aad_line, x), 'r')
```

```
plot(x, polyval(ave_line, x), 'k')
scatter(root, polyval(aad_line, root), 'r')
axis([-10 15 -450 550])

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('Slope')
ylabel('Percent Value')
legend('ADD%', 'Aveage Err', 'AAD "Fit"', 'Ave% "Fit"', strcat('@Slope = ',
num2str(root, 4')), 'Location', 'SouthEast')
hold off
```

Appendix D.2 – Viscosity Algorithm Code

```
%% INFORMATION
%
%  Combined GCSP program from the previous programs in order to graph the
%  data for reporting and presentations. It is also useful for spotting
%  coding errors and logic fallacies.
%
%  Matt Evanhoe, UDRI
%
%  The Calculation contained are based upon theory (mostly Teja and Rice) and
%  regression from other work done to compile this program.

%% DATA IMPORT AND CLEANING
clear all; close all; clc;

%Import all Information
builder_t = xlsread('builder.csv');
psuedo_group = xlsread('psuedo group mixed.csv');
ref_fluids = xlsread('ref fluids.csv');
crcden = xlsread('crcvis.csv');

%Matrix Sizing
[c,~] = size(psuedo_group);
[~,b] = size(ref_fluids);
[m,n] = size(builder_t);

%Removing Header from Samples
builder_nam = zeros(1,n);
builder_num = zeros(m-1,n);
for j = 2:m
   for i = 1:n
      builder_nam(i) = builder_t(1,i);
      builder_num(j-1, i) = builder_t(j,i);
   end
end
clear i j builder_t;
[m,n] = size(builder_num);

%Data File Cleaning
builder_temp = zeros(c,n);
for i = 1:n
   for j = 1:m
      if 33 >= j
         builder_temp(j,i) = builder_num(j,i);
```

```
        elseif j >= 34 && 49 >= j
            builder_temp(j+1,i) = builder_num(j,i) + builder_num(j+18,i);
        elseif j == 50
            builder_temp(51, i) = builder_num(j,i);
        elseif j == 51
            builder_temp(34, i) = builder_num(j,i);
        elseif j > 51 && j < 68

        elseif j >= 68 && j < 98
            builder_temp(j-16, i) = builder_num(j,i);
        elseif j == 98

        elseif j == 99
            builder_temp(j-17, i) = builder_num(j,i);
        elseif j == 100
            builder_temp(j-17, i) = builder_num(100, i) + builder_num(101,i);
        elseif j == 101

        else
            builder_temp(j-18, i) = builder_num(j,i);
        end
    end
end
builder_num = builder_temp;
clear m builder_temp;

%Pseudo-Critcial Values
num_comp = length(builder_num);
Mm = zeros(1,n);
acc = zeros(1,n);
Zcm = zeros(1,n);
mole_frac = zeros(num_comp, n);
for i = 1:n
    [Mm(i), ~, acc(i), Zcm(i), mole_frac(:,i), ~] = molecalc(builder_num(:,i).',
psuedo_group, num_comp);
end
clear builder_num

Vcm = zeros(1,n);
Vcm2 = zeros(1,n);
Tcm = zeros(1,n);
em = zeros(1,n);
kays_vcm = zeros(1,n);
kays_vcm2 = zeros(1,n);
kays_tcm = zeros(1,n);
for i = 1:n
```

```
   [Vcm(i), Tcm(i), em(i), ~, ~, ~] = rice_pseudocrit_simple(mole_frac(:,i).',
psuedo_group, num_comp, Mm(i), 0); %aij = 1
   Vcm2(i) = ((Vcm(i)*10^3)/Mm(i))^-1;

end
clear mole_frac psuedo_group num_comp

%%  DENSITY
t_C = zeros(n,3);
t_K = zeros(n,3);

for i = 1:n
   t_C(i,1) = -40;
   t_C(i,2) = -20;
   t_C(i,3) = 20;
   t_K(i,:) = t_C(i,:) + 273.15;
end
[~,f] = size(t_C);
clear t_C

runner = xlsread('runner_test.csv');
for k = 1:length(runner)

%Density - Teja & Rice - 1978'ish
rice_temp1 = runner(k,1); %n-octane
rice_temp2 = runner(k,2); %n-propylbenzene
rice_temp3 = 152; %n-decane
rice_temp4 = 1; %METHANE
rice_ref1 = zeros(1,b);
rice_ref2 = zeros(1,b);
rice_ref3 = zeros(1,b);
rice_ref4 = zeros(1,b);
for i=1:b
   rice_ref1(i) = ref_fluids(rice_temp1,i);
   rice_ref2(i) = ref_fluids(rice_temp2,i);
   rice_ref3(i) = ref_fluids(rice_temp3,i);
   rice_ref4(i) = ref_fluids(rice_temp4,i);
end
clear rice_temp1 rice_temp2 rice_temp3 rice_temp4;

t_Rden = zeros(n,f);
t_R2 = zeros(n,f);

delta_w = zeros(1,n);
pred_den_rice = zeros(n,f);
slope = zeros(n,f);
```

```
den_err_act = zeros(n,f);
pred_den_lk = zeros(n,f);
pred_den_cout = zeros(n,f);
pred_den_red = zeros(n,f);
pred_den_kays = zeros(n,f);
kays_red = zeros(n,f);
den_storage = zeros(n,f);

for i = 1:n
   for j = 1:f
      t_Rden(i,j) = t_K(i,j)/Tcm(i);

      %Teja & Rice Method
      delta_w(i) = (acc(i)-rice_ref1(6))/(rice_ref2(6)-rice_ref1(6));
      [pred_den_rice(i,j), slope(i,j)] = rice_pred_visR2(t_Rden(i,j), rice_ref1, rice_ref2,
em(i), delta_w(i));
      den_err_act(i,j) = ((crcden(i,j+1)-pred_den_rice(i,j))/pred_den_rice(i,j))*100;

      %Coutinho Method
      %pred_den_cout(i,j) = cout_pred_den(t_Rden(i,j), ref_fluids(4,:), ref_fluids(10,:),
ref_fluids(227,:), Vcm(i), Mm(i), acc(i));
      %err_cout(i,j) = ((crcden(i,2*j)-pred_den_cout(i,j))/pred_den_cout(i,j))*100;
      %pred_den_red3(i,j) = pred_den_cout(i,j)/Vcm2(i);

      %Reduced based on T-R Method
      pred_den_red(i,j) = pred_den_rice(i,j)/Vcm2(i);

      den_storage(i,j) = crcden(i,j+1);
   end
end

%AAD
point_err  = mean(mean(den_err_act));
ave_err(:,k) = mean(den_err_act);
%ave_errb = mean(mean(err_cout));
for i = 1:n
   for j = 1:f
      aad_sing(i,j) = abs(den_err_act(i,j)- point_err);
      %aad_cout_a(i,j) = abs(err_cout(i,j) - ave_errb);
   end
end
%aad_cout = sum(sum(aad_cout_a))/(n*f);


aad(k) = sum(sum(aad_sing))/(n*f);
slope_std = std(slope);
```

```
slope = mean(slope);
clear aad_sing

slope_out(:,k) = slope';
std_out(:, k) = slope_std';
end

root = -0.05;
l=1;
y=1;
for i = 1:length(runner)
   for j = 1:3
      plotter(l, :) = [aad(i), slope_out(j,i), ave_err(j,i), abs(aad(i)*ave_err(j,i)), i];

      t1 = slope_out(j,i);
      if t1 > (1.1*root) && t1 < (0.9*root)
         pairs(y, :) = [aad(i), slope_out(j,i), ave_err(j,i), i];
         y= y+1;
      else

      end
      l = l+1;
   end
end


crc_red = den_storage(40,3)/Vcm2(40);
crc_red2 = den_storage(40,3)/kays_vcm2(40);

[den_num, den_name] = xlsread('denlist.csv');
qq = length(den_num);
for i = 1:qq
   ref(i,:) = ref_fluids(den_num(i), :);
   [ref_den(i), red_den(i)] = den_calc(t_Rden(40,3), ref(i,:));
end
clear ref_fluids

%Regression Lines
x = linspace(-10,15);
aad_line = polyfit(plotter(:,2), plotter(:,1), 2);
ave_line = polyfit(plotter(:,2), plotter(:,3), 1);


%% PLOTS

%Info for xy-line
```

```
xyx = linspace(-10,10);
xyx25up = 0.975*xyx;
xyx25down = 1.025*xyx;

%Density Plots
crcden_store = zeros(n,f);
temp_store = zeros(n,f);
for i = 1:n
   for j = 1:f
   crcden_store(i,j) = crcden(i,j+1);
   temp_store(i,j) = crcden(i,j+1);
   end
end

den1 = reshape(pred_den_rice,1,n*f);
den2 = reshape(pred_den_lk,1,n*f);
%den3 = reshape(pred_den_cout,1,n*f);
den4 = reshape(pred_den_kays,1,n*f);
crc1 = reshape(crcden_store,1,n*f);
%clear crcden_store

%Teja/Rice
figure(1)
hold on
scatter(crc1, den1, 5, 'b', 'MarkerFaceColor', 'b')
plot(xyx, xyx25up, 'k--')
plot(xyx, xyx25down, 'k--')
plot(xyx,xyx)

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
axis([0 0.02 0 0.02])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('CRC Density Values')
ylabel('Model Predicted Values')
legend('Model A', '2.5% Error Lines', 'Location', 'NorthEast')
title('Teja/Rice')
hold off

%{
%Coutinho
figure(2)
hold on
scatter(crc1, den3, 5, 'b', 'MarkerFaceColor', 'b')
plot(xyx, xyx25up, 'k--')
plot(xyx, xyx25down, 'k--')
```

```
plot(xyx,xyx)

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
axis([0.7 0.95 0.7 0.95])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('CRC Density Values')
ylabel('Model Predicted Values')
legend('Model A', '2.5% Error Lines', 'Location', 'SouthEast')
title('Coutinho')
hold off
%}

figure(3)
hold on
scatter(ref(:,6), red_den)
scatter(acc(40), pred_den_red(40,3), 'r')
scatter(acc(40), crc_red, 'rd')
hold off

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('Acentric Factor')
ylabel('Reduced Density [g/cm^3]')
legend('Reference Fluids', 'Teja-Rice', 'CRC - Teja-Rice', 'Location', 'SouthEast')
hold off

figure(4)
hold on
scatter(plotter(:,2), plotter(:,1))
scatter(plotter(:,2), plotter(:,3))
plot(x, polyval(aad_line, x), 'r')
plot(x, polyval(ave_line, x), 'k')
scatter(root, polyval(aad_line, root), 'r')
axis([-10 15 -450 550])

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('Slope')
ylabel('Percent Value')
legend('ADD%', 'Aveage Err', 'AAD "Fit"', 'Ave% "Fit"', strcat('@Slope = ',
num2str(root, 4')), 'Location', 'SouthEast')
hold off
```

Appendix D.3 – Graphic Producing Code

```
%% INFORMATION
%
%  Combined GCSP program from the previous programs in order to graph the
%  data for reporting and presentations. It is also useful for spotting
%  coding errors and logic fallacies.
%
%  Matt Evanhoe, UDRI
%  Version 1.0 - 08/11/2014
%
%  The Calculation contained are based upon theory (mostly Teja and Rice) and
%  regression from other work done to compile this program.

%% DATA IMPORT AND CLEANING
clear all; close all; clc;

%Import all Information
builder_t = xlsread('builder.csv');
psuedo_group = xlsread('psuedo group mixed.csv');
ref_fluids = xlsread('ref fluids.csv');
crcden = xlsread('crc2.csv');
crcvis = xlsread('crcvis.csv');

%Matrix Sizing
[c,~] = size(psuedo_group);
[~,b] = size(ref_fluids);
[m,n] = size(builder_t);

%Removing Header from Samples
builder_nam = zeros(1,n);
builder_num = zeros(m-1,n);
for j = 2:m
   for i = 1:n
      builder_nam(i) = builder_t(1,i);
      builder_num(j-1, i) = builder_t(j,i);
   end
end
clear i j builder_t;
[m,n] = size(builder_num);

%Data File Cleaning
builder_temp = zeros(c,n);
for i = 1:n
   for j = 1:m
```

```
        if 33 >= j
            builder_temp(j,i) = builder_num(j,i);
        elseif j >= 34 && 49 >= j
            builder_temp(j+1,i) = builder_num(j,i) + builder_num(j+18,i);
        elseif j == 50
            builder_temp(51, i) = builder_num(j,i);
        elseif j == 51
            builder_temp(34, i) = builder_num(j,i);
        elseif j > 51 && j < 68

        elseif j >= 68 && j < 98
            builder_temp(j-16, i) = builder_num(j,i);
        elseif j == 98

        elseif j == 99
            builder_temp(j-17, i) = builder_num(j,i);
        elseif j == 100
            builder_temp(j-17, i) = builder_num(100, i) + builder_num(101,i);
        elseif j == 101

        else
            builder_temp(j-18, i) = builder_num(j,i);
        end
    end
end
builder_num = builder_temp;
clear m builder_temp;

%Pseudo-Critcial Values
num_comp = length(builder_num);
Mm = zeros(1,n);
acc = zeros(1,n);
Zcm = zeros(1,n);
mole_frac = zeros(num_comp, n);
for i = 1:n
    [Mm(i), ~, acc(i), Zcm(i), mole_frac(:,i), ~] = molecalc(builder_num(:,i).',
psuedo_group, num_comp);
end
clear builder_num

Vcm = zeros(1,n);
Tcm = zeros(1,n);
Tcm2 = zeros(1,n);
em = zeros(1,n);
for i = 1:n
```

```
   [Vcm(i), Tcm(i), em(i), ~, ~, ~] = rice_pseudocrit_simple(mole_frac(:,i).',
psuedo_group, num_comp, Mm(i), 0); %aij = 1
   [~, Tcm2(i), ~, ~, ~] = rice_pseudocrit2(mole_frac(:,i).', psuedo_group, num_comp,
Mm(i), 0); %aij < 1
end

mole_frac = [builder_nam; mole_frac];
xlswrite('mol_frac', mole_frac);
clear mole_frac psuedo_group num_comp

%%  DENSITY
t_C = zeros(n,6);
t_K = zeros(n,6);
for i = 1:n
   t_C(i,1) = crcden(i,3);
   t_C(i,2) = crcden(i,5);
   t_C(i,3) = crcden(i,7);
   t_C(i,4) = crcden(i,9);
   t_C(i,5) = crcden(i,11);
   t_C(i,6) = crcden(i,13);
   t_K(i,:) = t_C(i,:) + 273.15;
end
[~,f] = size(t_C);
clear t_C

%Density - Teja & Rice - 1978'ish
rice_temp1 = 2; %n-propylbenzene
rice_temp2 = 10; %n-decane
rice_ref1 = zeros(1,b);
rice_ref2 = zeros(1,b);
for i=1:b
   rice_ref1(i) = ref_fluids(rice_temp1,i);
   rice_ref2(i) = ref_fluids(rice_temp2,i);
end
clear rice_temp1 rice_temp2;

%Aij Model
Tcm3 = zeros(n,f);
for i =1:n
   for j = 1:f
      aij = (6.6743e-04*t_K(i,j))+0.7011; %Editted on 12/16/14 to reflect appropriate
regression method
      Tcm3(i,j) = aij*Tcm(i);
   end
end
clear aij
```

```
t_Rden = zeros(n,f);
t_Rden2 = zeros(n,f);
t_Rden3 = zeros(n,f);

delta_w = zeros(1,n);

pred_den_act = zeros(n,f);
den_err_act = zeros(n,f);

pred_den_aij = zeros(n,f);
den_err_aij = zeros(n,f);

pred_den_corr = zeros(n,f);
den_err_corr = zeros(n,f);

den_storage = zeros(n,f);

for i = 1:n
   for j = 1:f
      t_Rden(i,j) = t_K(i,j)/Tcm(i);
      t_Rden2(i,j) = t_K(i,j)/Tcm2(i);
      t_Rden3(i,j) = t_K(i,j)/Tcm3(i,j);

      delta_w(i) = (acc(i)-rice_ref1(6))/(rice_ref2(6)-rice_ref1(6));

      pred_den_act(i,j) = rice_pred_den(t_Rden(i,j), rice_ref1, rice_ref2, Vcm(i), Mm(i),
delta_w(i));
      den_err_act(i,j) = ((crcden(i,2*j)-pred_den_act(i,j))/pred_den_act(i,j))*100;

      pred_den_aij(i,j) = rice_pred_den(t_Rden2(i,j), rice_ref1, rice_ref2, Vcm(i), Mm(i),
delta_w(i));
      den_err_aij(i,j) = ((crcden(i,2*j)-pred_den_aij(i,j))/pred_den_aij(i,j))*100;

      pred_den_corr(i,j) = rice_pred_den(t_Rden3(i,j), rice_ref1, rice_ref2, Vcm(i),
Mm(i), delta_w(i));
      den_err_corr(i,j) = ((crcden(i,2*j)-pred_den_corr(i,j))/pred_den_corr(i,j))*100;

      den_storage(i,j) = crcden(i,2*j);
   end
end

%Correlation Lines between CRC and Models
modelA = polyfit(den_storage, pred_den_act, 1);
modelB = polyfit(den_storage, pred_den_aij, 1);
modelC = polyfit(den_storage, pred_den_corr, 1);
```

```
%Average Error
ave_err1 = mean(mean(den_err_act));
ave_err2 = mean(mean(den_err_aij));
ave_err3 = mean(mean(den_err_corr));

%Standard Deviation
stddev1 = std(reshape(pred_den_act, 1, n*f));
stddev2 = std(reshape(pred_den_aij, 1, n*f));
stddev3 = std(reshape(pred_den_corr, 1, n*f));

%AAD Stuff - AAD of the Error
aad1 = reshape(den_err_act, 1, n*f);
aad2 = reshape(den_err_aij, 1, n*f);
aad3 = reshape(den_err_corr, 1, n*f);

med1 = median(aad1);
med2 = median(aad2);
med3 = median(aad3);

aad1t = zeros(1,n*f);
aad2t = zeros(1,n*f);
aad3t = zeros(1,n*f);
for i = 1:(n*f)
   aad1t(i) = abs(aad1(i) - med1);
   aad2t(i) = abs(aad2(i) - med2);
   aad3t(i) = abs(aad3(i) - med3);
end
aad1 = sum(aad1t)/(n*f);
aad2 = sum(aad2t)/(n*f);
aad3 = sum(aad3t)/(n*f);
clear aad1t aad2t aad3t med1 med2 med3
%}
%%  VISCOSITY
%Temperature Inputs
t_C = zeros(n,3);
for i = 1:n
   t_C(i,:) = [-40, -20, 20];
   t_Kvis = t_C + 273.15;
end

%References for Viscosity
rice_temp1 = 82; %n-decane
rice_temp2 = 219; %1n-pentylbenzene
rice_ref1 = zeros(1,b);
rice_ref2 = zeros(1,b);
```

```
for i=1:b
   rice_ref1(i) = ref_fluids(rice_temp1,i);
   rice_ref2(i) = ref_fluids(rice_temp2,i);
end
clear ref_fluids rice_temp1 rice_temp2 b

%Aij Model
ff = 3;
Tcm4 = zeros(n,ff);
em2 = zeros(n,ff);
for i =1:n
   for j = 1:ff
      aij = ((-3.229*10^(-4))*t_Kvis(i,j))+1.1134;
      Tcm4(i,j) = aij*Tcm(i);
      em2(i,j) = (Vcm(i)^(2/3))*(Tcm4(i,j)^(-1/2))*(Mm(i)^(-1/2));
   end
end
clear aij

t_Rvis = zeros(n,ff);
t_Rvis2 = zeros(n,ff);
t_Rvis3 = zeros(n,ff);

pred_vis_act = zeros(n, ff);
vis_err_act = zeros(n,ff);
ln_vis_err_act = zeros(n,ff);

pred_vis_aij = zeros(n, ff);
vis_err_aij = zeros(n,ff);
ln_vis_err_aij = zeros(n,ff);

pred_vis_corr = zeros(n, ff);
vis_err_corr = zeros(n,ff);
ln_vis_err_corr = zeros(n,ff);
%Calculations
for i = 1:n
   for j = 1:ff
   t_Rvis(i,j) = t_Kvis(i,j)/Tcm(i);
   t_Rvis2(i,j) = t_Kvis(i,j)/Tcm2(i);
   t_Rvis3(i,j) = t_Kvis(i,j)/Tcm4(i,j);

   delta_w(i) = (acc(i)-rice_ref1(6))/(rice_ref2(6)-rice_ref1(6));

   [pred_vis_act(i,j)] = rice_pred_visR(t_Rvis(i,j), rice_ref1, rice_ref2, em(i), delta_w(i));
   [pred_vis_aij(i,j)] = rice_pred_visR(t_Rvis2(i,j), rice_ref1, rice_ref2, em(i),
delta_w(i));
```

```
   [pred_vis_corr(i,j)] = rice_pred_visR(t_Rvis3(i,j), rice_ref1, rice_ref2, em2(i,j),
delta_w(i));

   if t_C(i,j) == -40
      vis_err_act(i,j) = ((crcvis(i,2)-pred_vis_act(i,j))/pred_vis_act(i,j))*100;
      ln_vis_err_act(i,j) = abs((log(crcvis(i,2))-
log(pred_vis_act(i,j)))/log(pred_vis_act(i,j)))*100;
      vis_err_aij(i,j) = ((crcvis(i,2)-pred_vis_act(i,j))/pred_vis_act(i,j))*100;
      ln_vis_err_aij(i,j) = ((log(crcvis(i,2))-
log(pred_vis_act(i,j)))/log(pred_vis_act(i,j)))*100;
      vis_err_corr(i,j) = ((crcvis(i,2)-pred_vis_corr(i,j))/pred_vis_corr(i,j))*100;
      ln_vis_err_corr(i,j) = ((log(crcvis(i,2))-
log(pred_vis_corr(i,j)))/log(pred_vis_corr(i,j)))*100;
   elseif t_C(i,j) == -20
      vis_err_act(i,j) = ((crcvis(i,3)-pred_vis_act(i,j))/pred_vis_act(i,j))*100;
      ln_vis_err_act(i,j) = abs((log(crcvis(i,3))-
log(pred_vis_act(i,j)))/log(pred_vis_act(i,j)))*100;
      vis_err_aij(i,j) = ((crcvis(i,3)-pred_vis_act(i,j))/pred_vis_act(i,j))*100;
      ln_vis_err_aij(i,j) = ((log(crcvis(i,3))-
log(pred_vis_act(i,j)))/log(pred_vis_act(i,j)))*100;
      vis_err_corr(i,j) = ((crcvis(i,3)-pred_vis_corr(i,j))/pred_vis_corr(i,j))*100;
      ln_vis_err_corr(i,j) = ((log(crcvis(i,3))-
log(pred_vis_corr(i,j)))/log(pred_vis_corr(i,j)))*100;
   elseif t_C(i,j) == 20
      vis_err_act(i,j) = ((crcvis(i,4)-pred_vis_act(i,j))/pred_vis_act(i,j))*100;
      ln_vis_err_act(i,j) = abs((log(crcvis(i,4))-
log(pred_vis_act(i,j)))/log(pred_vis_act(i,j)))*100;
      vis_err_aij(i,j) = ((crcvis(i,4)-pred_vis_act(i,j))/pred_vis_act(i,j))*100;
      ln_vis_err_aij(i,j) = ((log(crcvis(i,4))-
log(pred_vis_act(i,j)))/log(pred_vis_act(i,j)))*100;
      vis_err_corr(i,j) = ((crcvis(i,4)-pred_vis_corr(i,j))/pred_vis_corr(i,j))*100;
      ln_vis_err_corr(i,j) = ((log(crcvis(i,4))-
log(pred_vis_corr(i,j)))/log(pred_vis_corr(i,j)))*100;
   else

   end

   end
end
clear rice_ref1 rice_ref2

vis_err = mean(mean(vis_err_act));
for i = 1:n
   for j = 1:ff
      aad_sing(i,j) = abs(vis_err_act(i,j) - vis_err);
   end
```

```
end
aad_vis = sum(sum(aad_sing))/(n*ff);

%% PLOTS
%
%Info for xy-line
xyx = linspace(-10,10);
xyx25up = 0.975*xyx;
xyx25down = 1.025*xyx;

%Density Plots
crcden_store = zeros(n,f);
temp_store = zeros(n,f);
for i = 1:n
   for j = 1:f
   crcden_store(i,j) = crcden(i,2*j);
   temp_store(i,j) = crcden(i,(2*j +1));
   end
end

den1 = reshape(pred_den_act,1,n*f);
den2 = reshape(pred_den_aij,1,n*f);
den3 = reshape(pred_den_corr,1,n*f);
crc1 = reshape(crcden_store,1,n*f);
%clear crcden_store

figure(1)
hold on
scatter(crc1, den1, 5, 'b', 'MarkerFaceColor', 'b')
%scatter(crc1, den2, 5, 'g^', 'MarkerFaceColor', 'g')
plot(xyx, xyx25up, 'k--')
plot(xyx, xyx25down, 'k--')
plot(xyx,xyx)

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
axis([0.7 0.95 0.7 0.95])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('CRC Density Values')
ylabel('Model Predicted Values')
legend('Prediction', '2.5% Error Lines', 'Location', 'SouthEast')
hold off
%{
%POSF 3962
figure(2)
hold on
```

```
scatter(temp_store(11,:), crcden_store(11,:), 12, 'g', 'MarkerFaceColor', 'g')
plot(temp_store(11,:), pred_den_act(11,:), 'b')
plot(temp_store(11,:), pred_den_aij(11,:), 'r')

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('Temperature (Celsius)')
ylabel('Density (g/cm^3)')
legend('Experiemental', 'Model A', 'Model B', 'Location', 'NorthEast')
hold off

%POSF 4158
figure(3)
hold on
scatter(temp_store(28,:), crcden_store(28,:), 12, 'g', 'MarkerFaceColor', 'g')
plot(temp_store(28,:), pred_den_act(28,:), 'b')
plot(temp_store(28,:), pred_den_aij(28,:), 'r')

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('Temperature (Celsius)')
ylabel('Density (g/cm^3)')
legend('Experiemental', 'Model A', 'Model B', 'Location', 'NorthEast')
hold off

%POSF 3896
figure(4)
hold on
scatter(temp_store(1,:), crcden_store(41,:), 12, 'g', 'MarkerFaceColor', 'g')
plot(temp_store(1,:), pred_den_act(41,:), 'b')
plot(temp_store(1,:), pred_den_aij(41,:), 'r')

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('Temperature (Celsius)')
ylabel('Density (g/cm^3)')
legend('Experiemental', 'Model A', 'Model B', 'Location', 'NorthEast')
hold off

figure(5)
hold on
scatter(crc1, den2, 12, 'g', 'MarkerFaceColor', 'g')
plot(xyx, xyx25up, 'k--')
```

```
plot(xyx, xyx25down, 'k--')
plot(xyx,xyx)
box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
axis([0.7 0.95 0.7 0.95])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('CRC Density Values')
ylabel('Model Predicted Values')
legend('Model B', '+- 2.5% Lines', 'Location', 'SouthEast')
hold off
%}

figure(6)
hold on
h = zeros(1,6);
%POSF 3896
h(1) = plot(temp_store(41,:), pred_den_act(41,:), 'r', 'LineWidth', 2);

%POSF 3962
h(2) = plot(temp_store(11,:), pred_den_act(11,:), 'b', 'LineWidth', 2);

%POSF 4158
h(3) = plot(temp_store(28,:), pred_den_act(28,:), 'k', 'LineWidth', 2);

h(4) = scatter(temp_store(41,:), crcden_store(41,:), 25, 'r^', 'MarkerFaceColor', 'r');
h(5) = scatter(temp_store(11,:), crcden_store(11,:), 35, 'bd', 'MarkerFaceColor', 'b');
h(6) = scatter(temp_store(28,:), crcden_store(28,:), 25, 'ko', 'MarkerFaceColor', 'k');

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('Temperature (°C)')
ylabel('Density (g/cm^3)')
legend(h(4:6),'POSF 3896 - JP-8', 'POSF 3962 - Jet-A', 'POSF 4158 - Jet A-1', 'Location',
'NorthEast')
hold off
clear h

%Viscosity Plots
crcvis_n = [crcvis(:,2),crcvis(:,3),crcvis(:,4)];
crc2 = reshape(crcvis_n,1,n*ff);
vis1 = reshape(pred_vis_act,1,n*ff);
vis2 = reshape(pred_vis_aij,1,n*ff);
vis3 = reshape(pred_vis_corr,1,n*ff);

logcrc = [log(crcvis(:,2)), log(crcvis(:,3)), log(crcvis(:,4))];
```

```
logcrc = abs(logcrc);
log_vis_act = log(pred_vis_act);
log_vis_act = abs(log_vis_act);
log_vis_aij = log(pred_vis_aij);
log_vis_aij = abs(log_vis_aij);
log_vis_corr = log(pred_vis_corr);
log_vis_corr = abs(log_vis_corr);

crc3 = reshape(logcrc, 1, n*ff);
vis4 = reshape(log_vis_act, 1, n*ff);
vis5 = reshape(log_vis_aij, 1, n*ff);
vis6 = reshape(log_vis_corr, 1, n*ff);
clear logcrc log_vis_act log_vis_aij log_vis_corr

crcvis_store = zeros(n,ff);
temp_store = [-40, -20, 20];
for i = 1:n
   for j = 1:ff
   crcvis_store(i,j) = crcvis(i,j+1);
   end
end

figure(10)
hold on
scatter(crc3, vis4, 12, 'b^', 'MarkerFaceColor', 'b')
plot(xyx, xyx25up, 'k--')
plot(xyx, xyx25down, 'k--')
plot(xyx,xyx)
box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
axis([4.0 7.0 4.0 7.0])
xlabel('Absolute Natural Log of CRC Viscosity Values')
ylabel('Absolute Natural Log of Model Predicted Values')
legend('Prediction', '+- 2.5% Lines', 'Location', 'SouthEast')
hold off

%{
figure(11)
hold on
scatter(crc3, vis4, 12, 'b^', 'MarkerFaceColor', 'b')
plot(xyx,xyx, 'r')
box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
axis([4.0 7.0 4.0 7.0])
```

```
xlabel('Absolute Natural Log of CRC Viscosity Values')
ylabel('Absolute Natural Log of Model Predicted Values')
legend('Model A', 'Location', 'SouthEast')
hold off


figure(12)
hold on
scatter(crc2, vis1, 20, 'b^', 'MarkerFaceColor', 'b')
plot(xyx,xyx, 'r')
box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
axis([0 14*10^-3 0 14*10^-3])
xlabel('CRC Viscosity Values')
ylabel('Model Predicted Values')
legend('Model A', 'Location', 'SouthEast')
hold off
%}
figure(13)
hold on

scatter(temp_store, crcvis_store(41,:), 25, 'b^', 'MarkerFaceColor', 'b')
scatter(temp_store, crcvis_store(11,:), 25, 'rd', 'MarkerFaceColor', 'r')
scatter(temp_store, crcvis_store(28,:), 25, 'go', 'MarkerFaceColor', 'g')

%POSF 3896
plot(temp_store, pred_vis_act(41,:), 'b', 'LineWidth', 2)

%POSF 3962
plot(temp_store, pred_vis_act(11,:), 'r', 'LineWidth', 2)

%POSF 4158
plot(temp_store, pred_vis_act(28,:), 'g', 'LineWidth', 2)

box
axis([-50 25 1*10^-3 11*10^-3])
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('Temperature (°C)')
ylabel('Viscosity (Pa*s)')
legend('POSF 3896 - JP-8', 'POSF 3962 - Jet-A', 'POSF 4158 - Jet A-1', 'Location',
'NorthEast')
hold off

temp_store_k = temp_store+273.15;
```

```
temp_store_i = 1./temp_store_k;
ln_crcvis_store = log(crcvis_store);
ln_pred_vis_act = log(pred_vis_act);

figure(14)
hold on

scatter(temp_store_i, ln_crcvis_store(41,:), 25, 'b^', 'MarkerFaceColor', 'b')
scatter(temp_store_i, ln_crcvis_store(11,:), 25, 'rd', 'MarkerFaceColor', 'r')
scatter(temp_store_i, ln_crcvis_store(28,:), 25, 'go', 'MarkerFaceColor', 'g')

%POSF 3896
plot(temp_store_i, ln_pred_vis_act(41,:), 'b', 'LineWidth', 2)

%POSF 3962
plot(temp_store_i, ln_pred_vis_act(11,:), 'r', 'LineWidth', 2)

%POSF 4158
plot(temp_store_i, ln_pred_vis_act(28,:), 'g', 'LineWidth', 2)

box
axis([3.25e-3 4.5e-3 -7 -4.5])
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 12, 'FontName', 'TimesNewRoman')
xlabel('1/T [K^-^1]')
ylabel('Natural Log of Viscosity [ln(Pa*s)]')
legend('POSF 3896 - JP-8', 'POSF 3962 - Jet-A', 'POSF 4158 - Jet A-1', 'Location',
'SouthEast')
hold off
%}
%% EXCEL INFO
%{
psuedo_out(1,:) = {'Fuel Number', 'Tcm (K)', 'Vcm (m^3/kmol)', 'Zcm', 'Accentric
Factor', 'Mmix (Kay"s)'};
for i=1:n
   psuedo_out(i+1, :) = {builder_nam(i), Tcm(i), Vcm(i), Zcm(i), acc(i), Mm(i)};
end

den_out(1,:) = {'Fuel Number', 'T (C)', 'Pred Den (g/cm^3)', 'T (C)',...
   'Pred Den (g/cm^3)', 'T (C)', 'Pred Den (g/cm^3)', 'T (C)',...
   'Pred Den (g/cm^3)', 'T (C)', 'Pred Den (g/cm^3)', 'T (C)', 'Pred Den (g/cm^3)'};
for i = 1:n
   den_out(i+1, :) = {builder_nam(i), crcden(i,3), pred_den_act(i,1), ...
      crcden(i,5), pred_den_act(i,2),crcden(i,7), pred_den_act(i,3),...
      crcden(i,9), pred_den_act(i,4),crcden(i,11), pred_den_act(i,5),...
      crcden(i,13), pred_den_act(i,6)};
```

```
end

vis_out(1,:) = {'Fuel Number', 'Pred Vis (Pa*s) @ -40 °C', 'Pred Vis (Pa*s) @ -20 °C',
'Pred Vis (Pa*s) @ 20 °C'};
for i = 1:n
    vis_out(i+1, :) = {builder_nam(i), pred_vis_act(i,1), pred_vis_act(i,2),
pred_vis_act(i,3)};
end

xlswrite('data_05_22_2015.xls', psuedo_out, 1)
xlswrite('data_05_22_2015.xls', den_out, 2)
xlswrite('data_05_22_2015.xls', vis_out, 3)
%}
```

Appendix D.4 – Subroutines Used in the Programs

Appendix D.4.1 – molecalc.m

```
function [a, b, c, d, e, f] = molecalc(x, y, z)
% Calculates the mole fraction, psuedo molecular weight (Kay's Rule), accentric factor
% (Kay's Rule), and compressibility factor (Kay's Rule) of each component.
sum_prod = 0;

%total mass
temp = zeros(1,z);
for i = 1:z
   temp(i) = (x(i)*y(i,3))/(12.0107*y(i,1));
   sum_prod = sum_prod + temp(i);
end

%Calculates the mass fraction and number of moles of each component
mass_frac = zeros(1,z);
moles = zeros(1,z);
for i = 1:z
   mass_frac(i) = temp(i)/sum_prod;
   moles(i) = mass_frac(i)/y(i,3);
end

a = 0; Mm2 = 0; c = 0; d = 0;
sum_moles = sum(moles);

e = zeros(1,z);
for i = 1:z
   e(i) = moles(i)/sum_moles;
   a = a + e(i)*y(i,3);
   Mm2 = Mm2 + e(i)*y(i,3)^2;
   c = c + e(i)*y(i,8);
   d = d + e(i)*y(i,7);
end

heat_com = zeros(1,z);
for i = 1:z
   heat_com(i) = e(i)*y(i,9);
end
f = sum(heat_com);

end
```

Appendix D.4.2 – rice_pseudocrit_simple.m

```
function [a, b, c, d, e, j] = rice_pseudocrit_simple(x, y, z, t, u)
%{
This function calculates psuedo-critical properties based upon Teja & Rice (1981). First
by calculating aij based on Prausnitz (1967) and Meng (2005). aij = 1 - kij.
%}

%Vcm
a = 0;
for i = 1:z
   for j = 1:z
      vij(i,j) = (1/8)*(y(i,6)^(1/3)+y(j,6)^(1/3))^3;
      vtv(i,j) = x(i)*x(j)*vij(i,j);
      a = a + vtv(i,j);
   end
end

clear i j;

%Tcm
tv = 0; b = 0;
for i = 1:z
   for j = 1:z
      tv = sqrt(y(i,4)*y(i,6)*y(j,4)*y(j,6));
      tij(i,j) = x(i)*x(j)*tv;
      b = b + tij(i,j);
   end
end
b = b/a;

%Viscosity
c = a^(2/3)*b^(-1/2)*t^(-1/2);

%Thermal Conductivity
d = a^(2/3)*b^(-1/2)*t^(1/2);

%Surface Tension (Pc)
j = 8.314*(0.291-(0.085*u))*(b/a);

e = j^(2/3)*b^(1/3);

end
```

Appendix D.4.3 – rice_pred_den.m

```
function [rho_out] = rice_pred_den(tr, ref1, ref2, v, m, w)
%Generalized Corresponding States Principle Density Prediction

temp = m/(10^3);
for i = 1:length(tr)
   a1 = tr(i)*ref1(2);
   b1 = (1-(a1/ref1(9)))^ref1(10);
   c1 = ref1(8)^(1+b1);
   d1 = ref1(7)/c1;
   v1 = 1/d1;
   inv1 = v1/ref1(4);

   a2 = tr(i)*ref2(2);
   b2 = (1-(a2/ref2(9)))^ref2(10);
   c2 = ref2(8)^(1+b2);
   d2 = ref2(7)/c2;
   v2 = 1/d2;
   inv2 = v2/ref2(4);

   rho_out(i) = temp*(v*(inv1+w*(inv2-inv1)))^-1;
end

end
```

Appendix D.4.4 – rice_pred_den2.m

```
function [rho_out, slope] = rice_pred_den2(tr, ref1, ref2, v, m, w)
%Generalized Corresponding States Principle Density Prediction

temp = m/(10^3);
for i = 1:length(tr)
   a1 = tr(i)*ref1(2);
   b1 = (1-(a1/ref1(9)))^ref1(10);
   c1 = ref1(8)^(1+b1);
   d1 = ref1(7)/c1;
   v1 = 1/d1;
   inv1 = v1/ref1(4);

   a2 = tr(i)*ref2(2);
   b2 = (1-(a2/ref2(9)))^ref2(10);
   c2 = ref2(8)^(1+b2);
   d2 = ref2(7)/c2;
   v2 = 1/d2;
   inv2 = v2/ref2(4);

   rho_out(i) = temp*(v*(inv1+w*(inv2-inv1)))^-1;
   slope = (inv2-inv1)/(ref2(6)-ref1(6));
end

end
```

Appendix D.4.5 – rice_pred_visR.m

```
function [rho_out, slope] = rice_pred_den2(tr, ref1, ref2, v, m, w)
%Generalized Corresponding States Principle Density Prediction

temp = m/(10^3);
for i = 1:length(tr)
   a1 = tr(i)*ref1(2);
   b1 = (1-(a1/ref1(9)))^ref1(10);
   c1 = ref1(8)^(1+b1);
   d1 = ref1(7)/c1;
   v1 = 1/d1;
   inv1 = v1/ref1(4);

   a2 = tr(i)*ref2(2);
   b2 = (1-(a2/ref2(9)))^ref2(10);
   c2 = ref2(8)^(1+b2);
   d2 = ref2(7)/c2;
   v2 = 1/d2;
   inv2 = v2/ref2(4);

   rho_out(i) = temp*(v*(inv1+w*(inv2-inv1)))^-1;
   slope = (inv2-inv1)/(ref2(6)-ref1(6));
end

end
```

Appendix D.4.6 – rice_pred_visR2.m

```
function [vis, slope] = rice_pred_visR2(tr, ref1, ref2, epi, w)
%Function to predict viscosity of a substance
vis = zeros(1,length(tr));
for i = 1:length(tr)
   a1 = ref1(13);
   b1 = ref1(14)/(tr(i)*ref1(2));
   c1 = ref1(15)*log(tr(i)*ref1(2));
   d1 = ref1(16)*((tr(i)*ref1(2))^ref1(17));
   ln_eta1 = a1 + b1 + c1 + d1;
   eta1 = exp(ln_eta1);
   epi1 = ref1(4)^(2/3)*ref1(2)^(-1/2)*ref1(1)^(-1/2);

   a2 = ref2(13);
   b2 = ref2(14)/(tr(i)*ref2(2));
   c2 = ref2(15)*log(tr(i)*ref2(2));
   d2 = ref2(16)*((tr(i)*ref2(2))^ref2(17));
   ln_eta2 = a2 + b2 + c2 + d2;
   eta2 = exp(ln_eta2);
   epi2 = ref2(4)^(2/3)*ref2(2)^(-1/2)*ref2(1)^(-1/2);

   step1 = (eta2*epi2)^w;
   step2 = (eta1*epi1)^(1-w);
   vis(i) = (step1*step2)/epi;
   slope = (ln_eta2-ln_eta1)/(ref2(6)-ref1(6));
end

end
```

Appendix D.4.7 – cout_pred_den.m

```
function [rho_out] = cout_pred_den(tr, ref1, ref2, ref3, v, m, w)
%Generalized Corresponding States Principle Density Prediction

temp = m/(10^3);
for i = 1:length(tr)
   a1 = tr(i)*ref1(2);
   b1 = (1-(a1/ref1(9)))^ref1(10);
   c1 = ref1(8)^(1+b1);
   d1 = ref1(7)/c1;
   v1 = 1/d1;
   inv1 = v1/ref1(4);

   a2 = tr(i)*ref2(2);
   b2 = (1-(a2/ref2(9)))^ref2(10);
   c2 = ref2(8)^(1+b2);
   d2 = ref2(7)/c2;
   v2 = 1/d2;
   inv2 = v2/ref2(4);

   a3 = tr(i)*ref3(2);
   b3 = (1-(a3/ref3(9)))^ref3(10);
   c3 = ref3(8)^(1+b3);
   d3 = ref3(7)/c3;
   v3 = 1/d3;
   inv3 = v3/ref3(4);

   D1 = (inv2-inv1)/(ref2(6)-ref1(6));
   D2a = (inv3-inv1)/(ref3(6)-ref1(6));
   D2 = (D2a - D1)/(ref3(6)-ref1(6));
   D3 = w - ref1(6);

   rho_out(i) = temp*(v*(inv1 + D1*D3 + D2*D3*(w-ref2(6))))^-1;
end

end
```

Appendix D.5 – Cleaned Up and Usable to Predict Values Code

```
%% INFORMATION
%
%  Combined GCSP program from the previous programs in order to graph the
%  data for reporting and presentations. It is also useful for spotting
%  coding errors and logic falicies.
%
%  Also, contains optimum 'Method 1' groups and fluids - see Evanhoe, M.
%  Thesis, University of Dayton, 2015
%
%  Matt Evanhoe, UDRI
%  Version 1.0 - 07/20/2015
%
%  The Calculation contained are based upon theory (for references see
%  above thesis) and regression from other work done to compile this program.

%% DATA IMPORT AND CLEANING
clear all; close all; clc;

%Import all Information
disp('Please select the fuel GCxGC csv file (press enter to continue):')
pause
input_file = uigetfile({'*.csv'; '*.xls'; '*.xlsx'});
fuel_num = input('Please input the POSF of the fuel you selected: ');
disp(' ')
disp('Importing file...')
disp(' ')
builder_t = xlsread(input_file);
psuedo_group = xlsread('psuedo group original.csv');
ref_fluids = xlsread('ref fluids.csv');

%Matrix Sizing
[c,~] = size(psuedo_group);
[~,b] = size(ref_fluids);
[m,n] = size(builder_t);

builder_num = builder_t;

%Data File Cleaning
builder_temp = zeros(c,n);
for i = 1:n
   for j = 1:m
      if 33 >= j
         builder_temp(j,i) = builder_num(j,i);
```

```
        elseif j >= 34 && 49 >= j
            builder_temp(j+1,i) = builder_num(j,i) + builder_num(j+18,i);
        elseif j == 50
            builder_temp(51, i) = builder_num(j,i);
        elseif j == 51
            builder_temp(34, i) = builder_num(j,i);
        elseif j > 51 && j < 68

        elseif j >= 68 && j < 98
            builder_temp(j-16, i) = builder_num(j,i);
        elseif j == 98

        elseif j == 99
            builder_temp(j-17, i) = builder_num(j,i);
        elseif j == 100
            builder_temp(j-17, i) = builder_num(100, i) + builder_num(101,i);
        elseif j == 101

        else
            builder_temp(j-18, i) = builder_num(j,i);
        end
    end
end
builder_num = builder_temp;
clear m builder_temp;

builder_num = builder_num(:,3);
[~, n] = size(builder_num);

disp('File Import and Cleaning Complete...')
disp(' ')
disp('Calculating Molecular Weight, Mole Fractions, and Critical Properties...')
disp(' ')

%Pseudo-Critcial Values
num_comp = length(builder_num);
mole_frac = zeros(num_comp, n);
[Mm, ~, acc, Zcm, mole_frac(:), ~] = molecalc(builder_num(:), psuedo_group,
num_comp);
clear builder_num

[Vcm, Tcm, em, ~, ~, ~] = rice_pseudocrit_simple(mole_frac(:), psuedo_group,
num_comp, Mm, 0);
clear mole_frac psuedo_group num_comp

disp('Calculations Complete...')
```

```
disp(' ')

%%  DENSITY
disp('Density Input and Calculations');
disp(' ');
t1 = input('Please the lowest temperature you wish to calculate (in °C): ');
t2 = input('Please the highest temperature you wish to calculate (in °C): ');
t_step = input('Please the temperature step you wish to calculate (in °C): ');
disp(' ')
disp('Calculating Temperatures...')

t_points = ((t2-t1)/t_step)+1;
t_C = linspace(t1, t2, t_points);
tt = length(t_C);
clear t1 t1 t_step t_points
disp(['Temperatures: ', num2str(t_C)]);
disp(' ');

t_K = zeros(1,tt);
for i = 1:tt
   t_K(i) = t_C(i) + 273.15;
end
f = length(t_C);
clear t_C

%Density - Teja & Rice - 1978'ish
rice_temp1 = 2; %ethane
rice_temp2 = 10; %isopentane
rice_ref1 = zeros(1,b);
rice_ref2 = zeros(1,b);
for i=1:b
   rice_ref1(i) = ref_fluids(rice_temp1,i);
   rice_ref2(i) = ref_fluids(rice_temp2,i);
end
clear rice_temp1 rice_temp2;

%Aij Model
t_Rden = zeros(n,f);
delta_w = zeros(1,n);
pred_den_act = zeros(n,f);
den_err_act = zeros(n,f);
for j = 1:f
   t_Rden(j) = t_K(j)/Tcm;
   delta_w = (acc-rice_ref1(6))/(rice_ref2(6)-rice_ref1(6));
   pred_den_act(j) = rice_pred_den(t_Rden(j), rice_ref1, rice_ref2, Vcm, Mm, delta_w);
end
```

```
disp('Density Successfully Calculated...');
disp(' ');

%%  VISCOSITY
%Temperature Inputs
disp('ViscosityInput and Calculations');
disp(' ');
t1 = input('Please the lowest temperature you wish to calculate (in °C): ');
t2 = input('Please the highest temperature you wish to calculate (in °C): ');
t_step = input('Please the temperature step you wish to calculate (in °C): ');
disp(' ')
disp('Calculating Temperatures:')

t_points = ((t2-t1)/t_step)+1;
t_C2 = linspace(t1, t2, t_points);
tt = length(t_C2);
clear t1 t1 t_step t_points
disp(['Temperatures: ', num2str(t_C2)]);
disp(' ');

t_Kvis = zeros(1,n);
for i = 1:tt
   t_Kvis(i) = t_C2(i) + 273.15;
end
ff = length(t_C2);
clear t_C2

%References for Viscosity
rice_temp1 = 87; %n-propylbenzene
rice_temp2 = 119; %n-butylbenzene
rice_ref1 = zeros(1,b);
rice_ref2 = zeros(1,b);
for i=1:b
   rice_ref1(i) = ref_fluids(rice_temp1,i);
   rice_ref2(i) = ref_fluids(rice_temp2,i);
end
clear ref_fluids rice_temp1 rice_temp2 b


t_Rvis = zeros(n,ff);
pred_vis_act = zeros(n, ff);
%Calculations
for j = 1:ff
   t_Rvis(j) = t_Kvis(j)/Tcm;
```

```
    delta_w = (acc-rice_ref1(6))/(rice_ref2(6)-rice_ref1(6));

    pred_vis_act(j) = rice_pred_visR(t_Rvis(j), rice_ref1, rice_ref2, em, delta_w);

end
clear rice_ref1 rice_ref2

disp('Viscosity Successfully Calculated...');
disp(' ');

%% PLOTS

%Density Plots
figure(1)
hold on
scatter(t_K, pred_den_act, 5, 'b^', 'MarkerFaceColor', 'b')
plot(t_K, pred_den_act, 'b')

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 10, 'FontName', 'TimesNewRoman')
xlabel('Temperature [K]')
ylabel('Model Predicted Values [g/mL]')
legend(num2str(fuel_num), 'Location', 'NorthEast')
hold off


%Viscosity Plots
vis1 = reshape(pred_vis_act,1,n*ff);
log_vis_act = log(pred_vis_act);
log_vis_act = abs(log_vis_act);
vis4 = reshape(log_vis_act, 1, n*ff);
clear log_vis_act

figure(2)
hold on
scatter(t_Kvis, pred_vis_act, 12, 'b^', 'MarkerFaceColor', 'b')
plot(t_Kvis, pred_vis_act, 'b')

box
set(gca, 'units', 'inches', 'position', [0.75 0.5 4.5 3.5])
set(gca, 'FontSize', 10, 'FontName', 'TimesNewRoman')
xlabel('Temperature [K]')
ylabel('Model Predicted Values [Pa*s]')
legend(num2str(fuel_num), 'Location', 'NorthEast')
hold off
```

```
%% EXCEL INFO

data_out(1,:) = {'Fuel Number', 'Tcm (K)', 'Vcm (m^3/kmol)', 'Accentric Factor', 'Mmix
(Kay''s)'};
data_out(2,:) = {fuel_num, Tcm, Vcm, acc, Mm};
data_out(4,:) = {'Density [g/mL]', 'Temperature [K]', ' ', ' ', ' '};

for i = 1:f
   data_out(i+4, :) = {pred_den_act(i), t_K(i), ' ', ' ', ' '};
end

data_out(f+6,:) = {'Dynamic Viscosity [Pa*s]', 'Temperature [K]', ' ', ' ', ' '};
for i = 1:ff
   data_out(i+f+6, :) = {pred_vis_act(i), t_K(i), ' ', ' ', ' '};
end

fileout = strcat('POSF_', num2str(fuel_num));
xlswrite(fileout, data_out)

disp(['All calculations complete and the data written to ', fileout, '.xls'])
disp('Thank you for using our program.')
```